# Interface Engineering of Perovskite Solar Cells using Mg-doped ZnO as Electron Selective Layers

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## Introduction

Recently, perovskite solar cell has attracted much attention as a next generation solar cell. In the solar cells, besides absorber layer material, the electron-selective layer (ESL) material is also very important. The ESL is not only crucial to achieving high photovoltaic conversion efficiency (PCE), but also for the device stability. Compared with other metal oxide, ZnO is particularly promising act as ESL, because of its high transparency, suitable work function, and high electron mobility. In addition, low-content doping/modification of metal oxides has been considered as a way of improving the selectivity of ESLs. Here, we have applied Zn<sub>1-x</sub>Mg<sub>x</sub>O as ESL in MAPbI<sub>3</sub> perovskite solar cells. We find that the conduction band edge position of the Zn<sub>1-x</sub>Mg<sub>x</sub>O layer can be tuned upward continuously via increasing x, and the photovoltaic performance, especially Voc depends greatly on x. The devices based on Zn<sub>0.9</sub>Mg<sub>0.1</sub>O ESL exhibited the best photovoltaic performance and a PCE of ~15.5% was achieved. The mechanism of the effects of the Zn<sub>1-x</sub>Mg<sub>x</sub>O ESLs on the PECs will be discussed.

### **Experimental Method**

The perovskite (MAPbI<sub>3</sub>) films were deposition according to a modified literature method.<sup>1</sup> Zn<sub>1-x</sub>Mg<sub>x</sub>O layer were prepared by sol–gel method. The precursor was prepared by employing zinc acetate dehydrate and magnesium acetate tetrahydrate (0%, 5%, 10%, and 20% mol) as Zn and Mg source, respectively. The sol-precursor was spin coated at 3000 rpm for 30 s on FTO glass substrate, then annealed in oven at 290 °C for 30 min. Then, Zn<sub>1-x</sub>Mg<sub>x</sub>O compact film was coated with MAPbI<sub>3</sub>. Finally, the device was then completed with an Au contact deposited via a shadow mask resulting in a device of area 0.16 cm<sup>2</sup>.

#### **Results and Discussion**

The addition of Mg can either replace  $Zn^{2+}$  or form MgO secondary phase. From XPS results, we observed that the binding energy peaks related to Mg 2p, as well as Zn 2p and O 1s, appeared for all Mg doped samples, demonstrating the successful doping of Mg elements and the formation of ternary oxide films of Zn<sub>1-x</sub>Mg<sub>x</sub>O. But when x =0.2, the binding energy peak Mg 2P and Oxygen 1s position have changed, indicating addition of Mg may form MgO phase.

Figure 1(a). shows the photovoltaic performance of the perovskite solar cells with Zn1-xMgxO ESLs for different x. It can be observed that Voc, Jsc and FF increase with x increasing from 0 to 0.1 and then decrease again as x increases further up to 0.2. To investigate the mechanism, we characterized the charge carrier lifetime of the solar cells by measuring the Voc decay. As shown in Figure 1(b), the photovoltage-dependent effective carrier lifetime becomes longer as x increases from 0 to 0.1, and then becomes shorter with x increases up to 0.2. These results indicate that the interfacial recombination at the Zn<sub>1-x</sub>Mg<sub>x</sub>O /MAPbI<sub>3</sub> interface depends strongly on the property of the Zn1-xMgxO ESLs. Two possible reasons can be considered about it. First, the conduction band edge of Zn<sub>1-x</sub>Mg<sub>x</sub>O became higher as x increasing as shown in the inset of Fig. 1(a), so the Voc increases and the recombination between injected electrons and holes remained in perovskite can be reduced greatly. Secondly, we have observed that PL intensity related to the



Figure 1. (a) J-V characteristics under simulated AM1.5G illumination (The inset shows an increase in the bandgap of  $Zn_{1-x}Mg_xO$  films). and (b) The effective carrier lifetimes calculated from the voltage decay curves.

trapping states in the ZnO layers decreases with x increasing up to 0.1 and then increases again as x increasing from 0.1 to 0.2. It means that the concentration of trapping states in ZnO decreases as Mg is doping and becomes is the smallest when x is 0.1, but it increases when more Mg is doping in the case of x>0.1. Therefore, benefiting from the reduced interfacial charge recombination and the reduced trapping states for x=0.1, a maximum efficiency of 14.01% (0.16 cm<sup>2</sup>) has been achieved, which is 30% higher compared to that of the devices without Mg doping ( $\eta$ =10.51%). And then, due to further optimization, a champion device with the PCE of 15.5 % was achieved. These results clearly indicate a potential avenue for the fabrication of perovskite solar cells with high efficiency by introducing a ZnMgO-ESLs with the possibility of interface modification engineering.

#### References

1. H.Zhang et al., Adv. Energy Mater. 2015, 5, 1501354.