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$MgCl_2$ Passivated ZnO Electron Transporting Layer to Improve PbS Quantum Dot Solar Cells

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Abstract: The unique tunable bandgaps and straightforward synthesis of colloidal quantum dots make them promising low-cost materials for photovoltaics. High-performance colloidal quantum dot solar cells rely on good-quality electron transporting layers to make carrier selective contacts. Despite extensive use of n-type oxides as electron transporting layers, a detailed understanding of their surface and interface states as well as mechanisms to improve their optical properties are still under development. Here, we report a simple procedure to produce $MgCl_2$ passivated ZnO nanoparticles electron transporting layers that show improved device performance. The $MgCl_2$ treated ZnO electron transporting layers boost the PbS colloidal quantum dot cell efficiency from 6.3% to 8.2%. The cell exhibits reduced defects leading to significant improvements of both FF and J_{sc}. This low-temperature $MgCl_2$ treated ZnO electron transporting layer may be applied in solution processed tandem cells as a promising strategy to further increase cell efficiencies.

In this research, a simple $MgCl_2$ treatment was introduced to passivate ZnO electron transporting layer and to further improve quantum dot solar cells' performance. $MgCl_2$ solution was added to ZnO nanoparticles solution drop-wisely making a ratio of Mg : Zn = 1 : 50 as shown in Figure 1a. X-ray photoelectron spectroscopy (XPS) shows the successful incorporation of Mg and Cl elements as in Figure 1b and 1c.

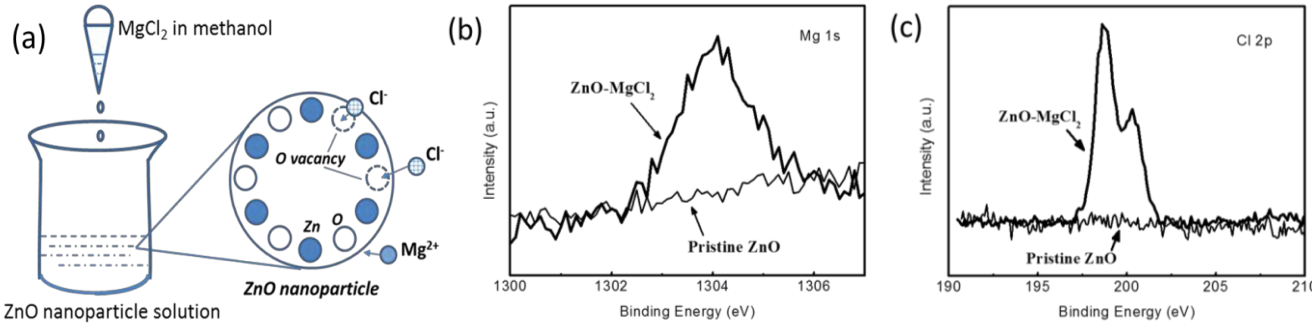

Figure 1 (a) Illustration of $MgCl_2$ treatment on ZnO nanoparticles in a solution and demonstration of defects elimination. $MgCl_2$ is added to ZnO nanoparticle solution at ambient temperature. Cl^- can occupy surface oxygen vacancies while Mg^{2+} may form Mg-O bonds on the nanoparticle surface. (b) XPS data of the Mg 1s peak for both pristine ZnO and ZnO-$MgCl_2$ films. (c) XPS peak of Cl 2p of both pristine ZnO and ZnO-$MgCl_2$ films.

By this simple one chemical treatment two effects, reduction in defects and increased transparency, were achieved. To verify the surface defect reduction, photoluminescence spectra with an excitation wavelength of 325 nm were measured for both pristine ZnO and ZnO-$MgCl_2$ samples. In Figure 2a, the broad emission peak at 550 nm (2.25 eV) is attributed to defect emission from deep levels in the bandgap.[1-4] The decrease in this defect emission peak indicates a reduction in surface defects due to the $MgCl_2$ treatment. Also, increasing the transparency of ZnO layers by introducing Mg is another motivation behind this research.[5, 6] With the very small amount of $MgCl_2$ incorporated into the synthesis, an increase of approximately 3% in transmission was observed from $MgCl_2$ treated ZnO films as shown in Figure 2b.

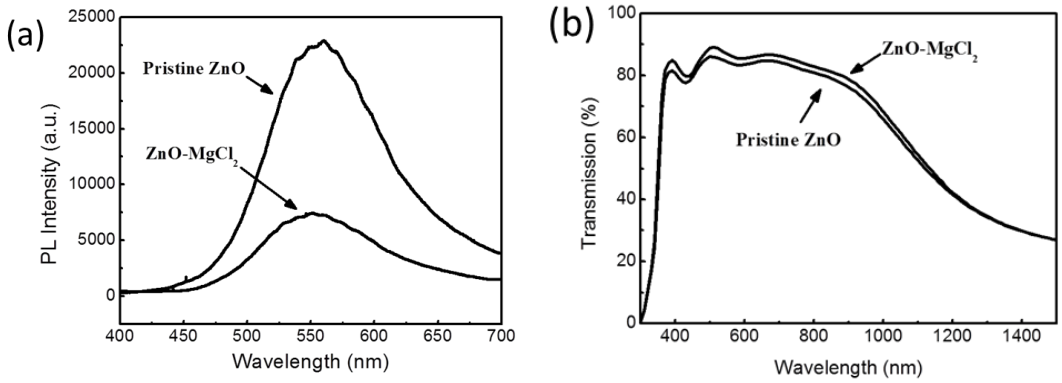

Figure 2 (a) Defect PL spectra of pristine ZnO and ZnO-$MgCl_2$ films. The reduction in the peak intensity between 450 nm and 700 nm is attributed to a reduction of surface defects. (b) Transmission of both ZnO-$MgCl_2$ and pristine ZnO films.

The fabricated PbS CQD solar cells are in the structure of glass/ITO/ZnO-$MgCl_2$/PbS-I/PbS-EDT/Au (See cross-sectional SEM image in Figure 3a). The J-V curves of the PbS CQD solar cells are shown in Figure 3b. An 8.2% PCE was achieved by using $MgCl_2$ treated ZnO, compared to the 6.3% PCE of the control cell using pristine ZnO. This increase is mainly attributed to an increase of the FF. A FF of 62% was achieved using $MgCl_2$ treated ZnO, compared to 53% FF of the cell using pristine ZnO. An increase in J_{sc} also contributes to the increased device efficiency.

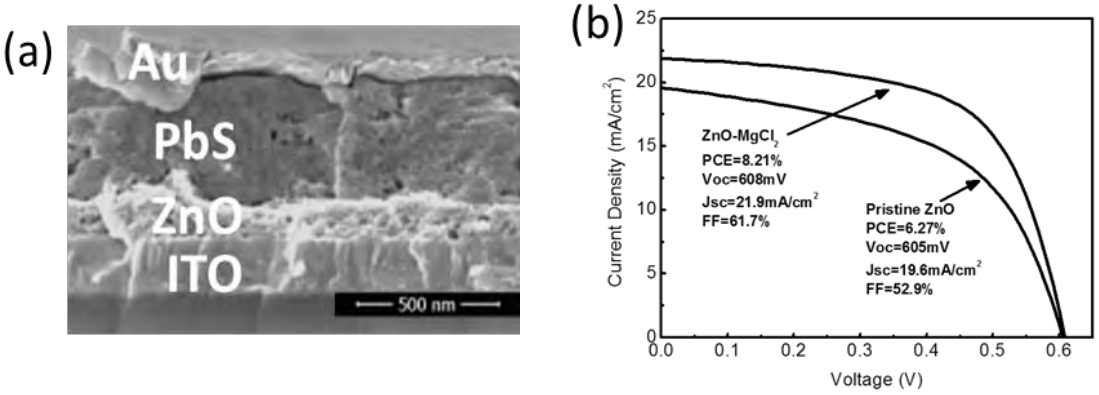

Figure 3 (a) SEM cross-sectional image of a PbS CQD solar cell with a glass/ITO/ZnO-$MgCl_2$/PbS-I/PbS-EDT/Au layer stack. The thickness of the ZnO film is 120 nm, the PbS-I CQD film is ~280 nm and the PbS-EDT layer is ~100 nm. (b) The J-V curves of the cell using ZnO-$MgCl_2$ and a control cell using pristine ZnO.

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