Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Charge Transfer Induced Photoluminescence in ZnO Nanoparticles

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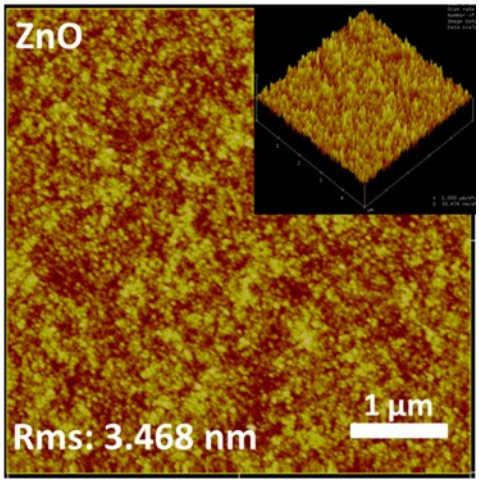

Figure S1. Atomic force microscopy (AFM) topography (5 × 5µm) of ZnO film. The scale bar: 1µm.

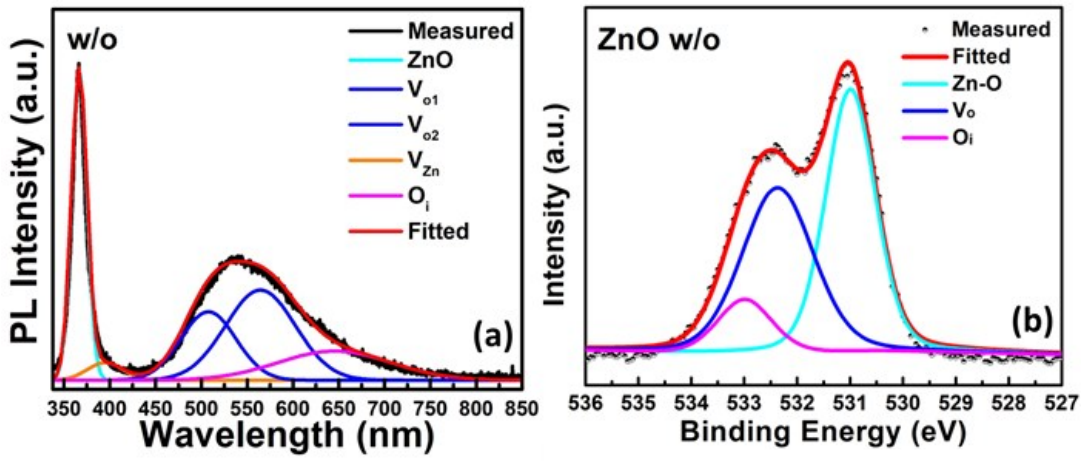

Figure S2. Previously reported defect analysis approach: Gaussian fitting of (a) ZnO NP film PL spectrum, and (b) high-resolution XPS spectrum of O 1s ZnO NP film.

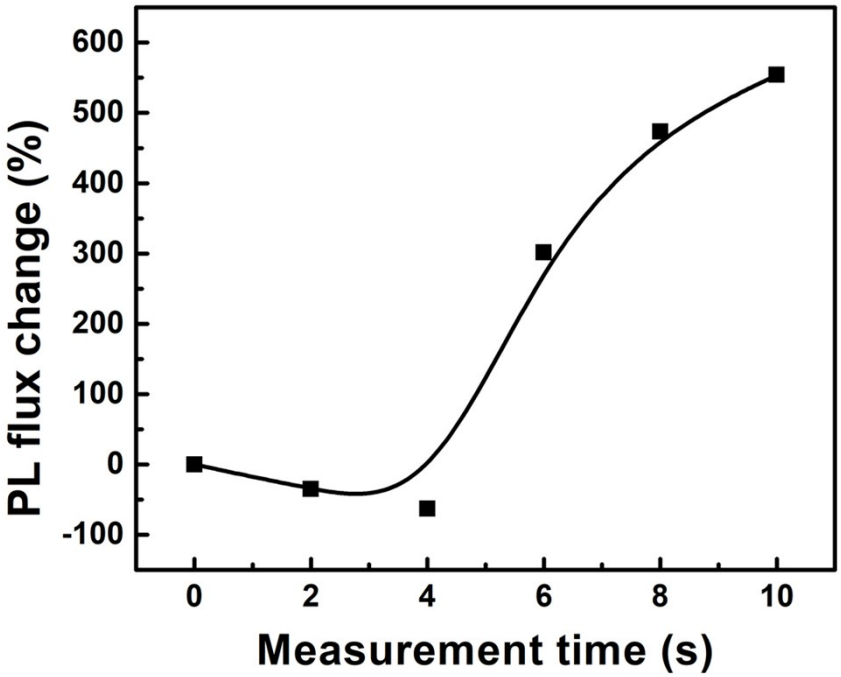

Figure S3. The calculated PL flux change at different exposure time in O_2 with respective to the PL flux at t = 0.

The PL photon flux at different exposure time, $Flux_t$, is calculated with the data shown in Figure 2 (b) and the calibrated responsivity of the CCD array (flux/count) using the following equation.

$$\frac{Flux_t - Flux_{t=0}}{Flux_{t=0}} \times 100\% \qquad (1)$$

This result shows the relative change of photon flux with respect to the flux at t = 0. It gives the estimation of the change of PL quantum yield.

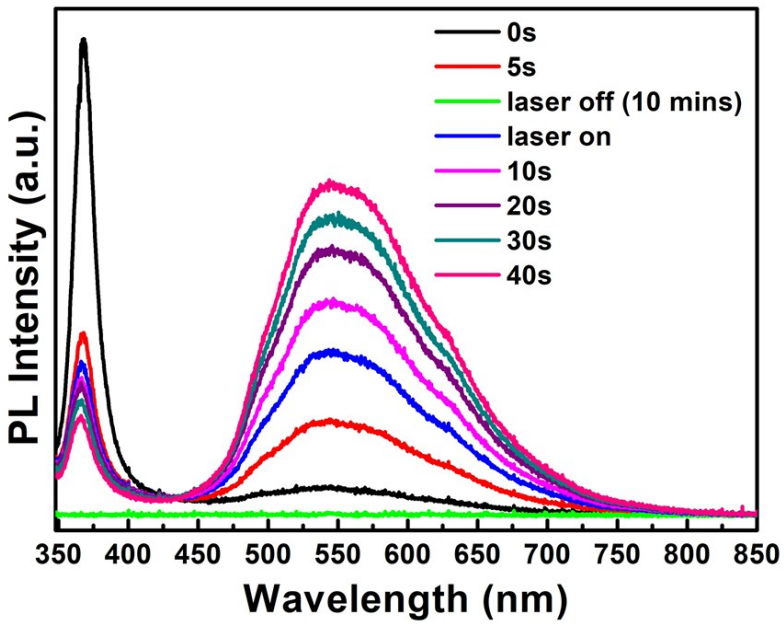

Figure S4. PL spectrum of ZnO NP thin film with excitation laser cut off for 10 minutes and on.

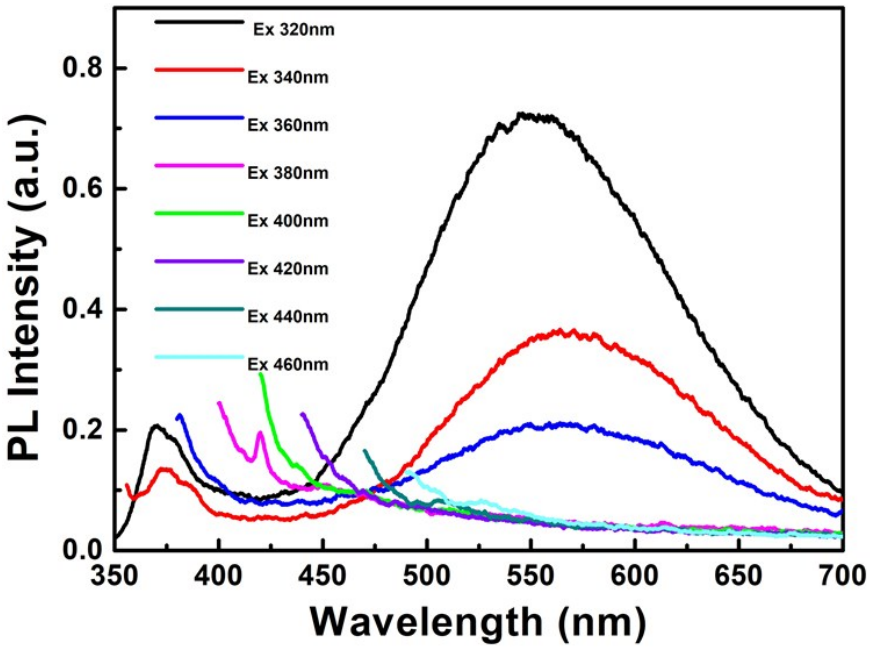

Figure S5. Excitation dependent PL of ZnO NP thin film with every 20 nm interval wavelength. The visible emission can only be observed with above bandgap (<360 nm) excitation.

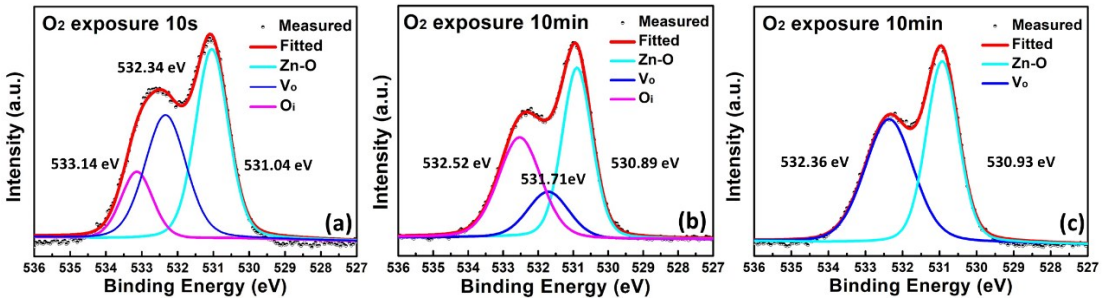

Figure S6. Gaussian fitting of XPS spectra of ZnO film with O_2 exposure for (a) 10 s and (b) and (c) 10 min.

According to the most widely adopted approach reported in literatures, the O 1s peak can be deconvolved into three peaks corresponding to the binding energies of oxygen of Zn-O (531eV), oxygen vacancy V_O (532 eV), and oxygen interstitial O_i (533eV). However, we have found that the analysis by peak fitting is not reliable, and even contradictory.

For example, when comparing the 10 s and 10 mins UV+O_2 exposed samples as shown in Figure S6, the peak fitting has multiple solutions. One solution (Figure S6b) suggests an reduce of V_o and increase of O_i, another solution (Figure S6c) on the other hand suggests an increase of V_o and reduce of O_i. Consequently, such multiple solutions from peak fitting have also been found in other samples.