## **Supplementary Material**

## Spectroscopic evidence for Li doping creation shallow $\mathbf{V}_{Zn}$ in

## ZnO

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Supplementary information:

ZnO nanoparticles with mean particle sizes in the range of 50~90 nm (Sigma-Aldrich, 99.99%) were also employed to verify the reproducibility of the 3 eV emission induced by  $H_2O_2$  oxidation. As shown in Figure.S1, treating with diluted  $H_2O_2$  solution (6 wt %) suppressed donor defects and produced the 414 nm emission. Further increase  $H_2O_2$  solution concentration to above 10 % can fully remove the donor-bound exciton at 368 nm and generated the deep level emission at 550 nm. These phenomena apparently demonstrate that abundant  $V_{Zn}$  were created after  $H_2O_2$  treatment.



Fig. S1. 10 K PL spectra of pristine 90 nm ZnO (a), treated with 6 %  $H_2O_2$  (b) and 30%  $H_2O_2$  solution (c). The inset shows the corresponding PLE spectra for the green emission. All of the

spectra are recorded at 10 K.