Supporting Information

Bulk and Surface Excitons in Alloyed and Phase–Separated Zn–Mg–O Particulate Systems

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Enclosure:

Description for calculating the chemical formula of the periclase–phase solid–solution and three figures.

Calculation of the chemical formula of the periclase–phase solid solution:

From Rietveld refinement, a weight percentage of the wurtzite phase of 5.9% is estimated. We assume the wurtzite phase consists of only ZnO, while the periclase phase contains both Zn and Mg. Starting with 0.3 mol of ZnO and 0.7 mol of MgO as determined by the precursor solution design, the mass of wurtzite ZnO is:

$$(0.3\times81.41+0.7\times40.30)\times5.9\%=3.11(\text{g})$$

The rest of the total mass is in the periclase phase:

$$(0.3\times81.41+0.7\times40.30)\times94.1\%=49.53\ (\text{g})$$

The molar ratio between Zn and Mg is the periclase phase is:

$$\left(\frac{0.3\times81.41-3.11}{81.41}\right)/0.7=0.26/0.7$$

The formula of the periclase phase compound is:

$Zn_{0.26}Mg_{0.7}O_{0.96}$, or $Zn_{0.27}Mg_{0.73}O$.

The formula weight of the periclase phase compound is then 51.39 g mol^{-1}.

Therefore, the molar ratio between the wurtzite and the periclase phase is:

$$\left(\frac{3.11}{81.41}\right)/\left(\frac{49.53}{51.39}\right)=1/25$$

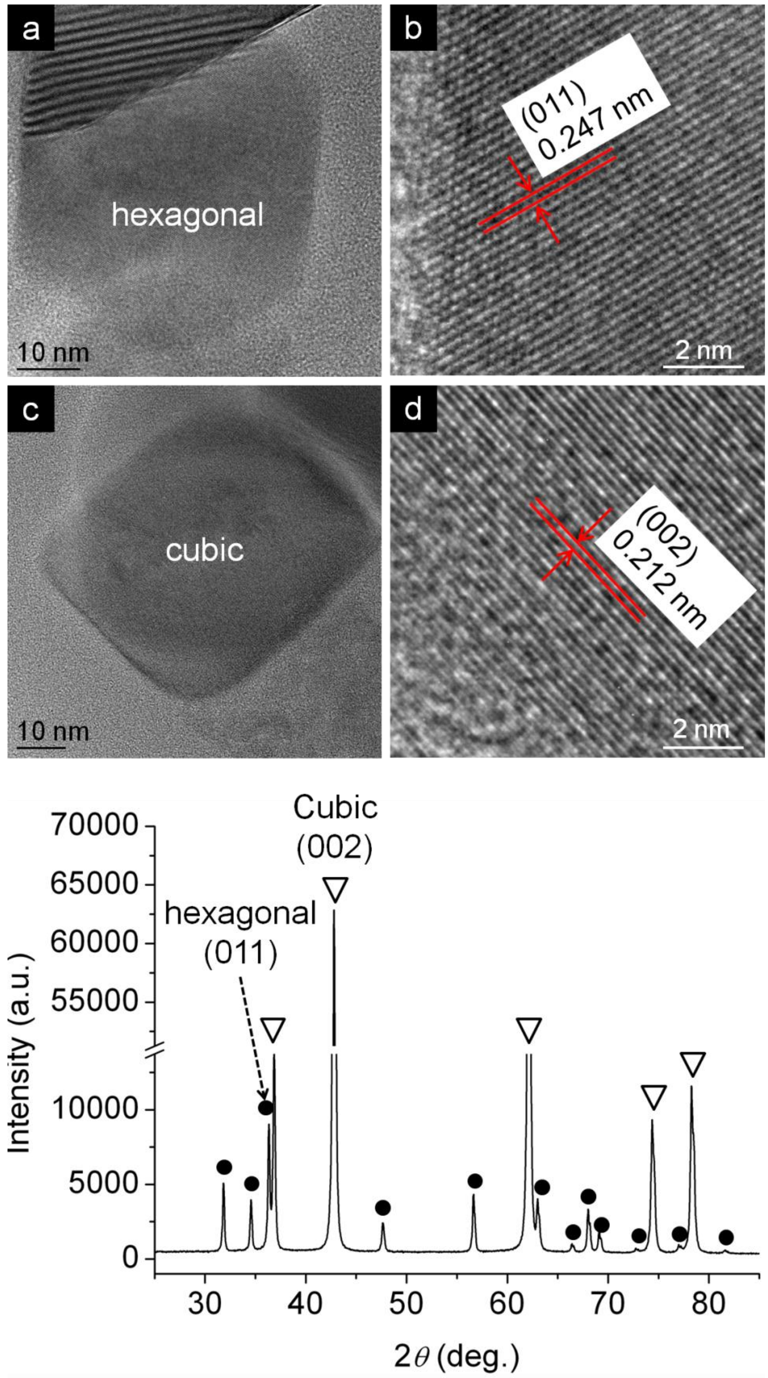

Figure S1. TEM images and XRD patterns showing different crystalline domains in the vacuum annealed $Zn_{0.3}Mg_{0.7}O$ sample. The measured distances of 0.247 nm (b) and 0.212 nm (d) correspond to the (011) and (002) *d*–spacings in the hexagonal (a, b) and cubic (c, d) domains, respectively. The (011) and (002) planes correspond to the strongest reflections in the XRD patterns of the wurtzite (solid circles) and the periclase (empty triangles) phases.

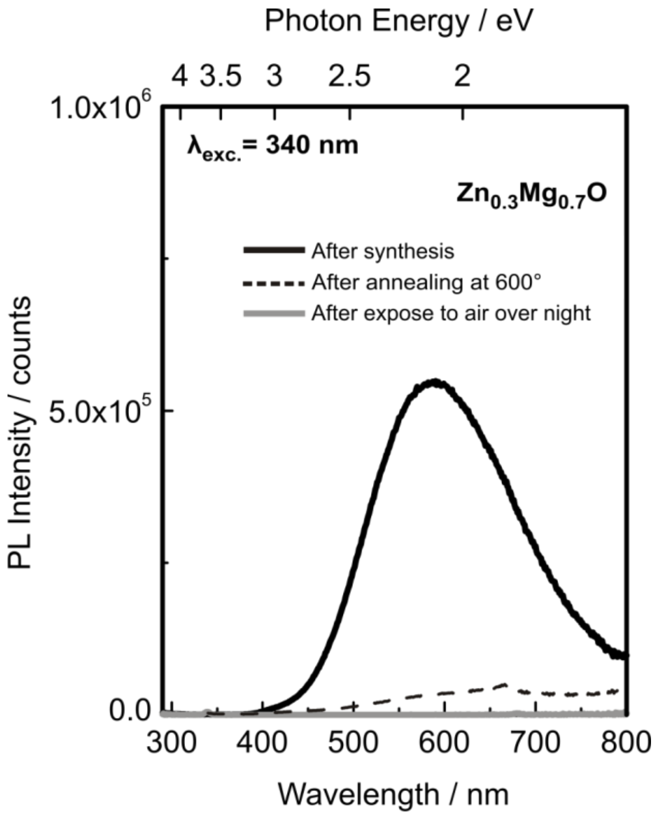

Figure S2. Effects of annealing and exposure to air/O_2 atmosphere on the PL emission properties of the $Zn_{0.3}Mg_{0.7}O$ sample. The annealing time is 30 minutes.

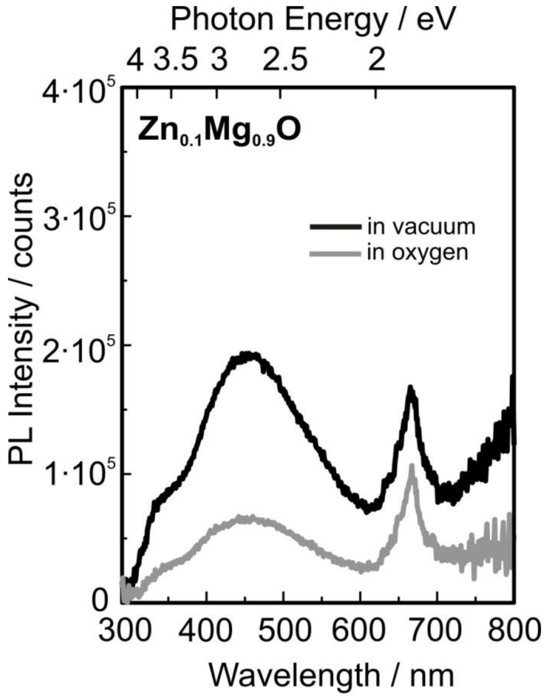

Figure S3. Room temperature photoluminescence emission spectra ($\lambda_{exc.}$ = 340 nm) of hydroxylated $Zn_{0.1}Mg_{0.9}O$ nanoparticle powders after vacuum annealing and oxidation at T = 873 K. Different to samples with entirely dehydroxylated particle surfaces molecular oxygen does not entirely quench the PL emission band at 2.8 eV which indicates that surface hydroxyls counteract energy transfer between photoexcited surface states and molecular oxygen.