# Electronic Supplementary Information (ESI)

# Impact of Band-gap Graded Structures Artificially Implemented in Mg-ZnO Epitaxial Films on Photoelectrochemical Properties

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| | Sample Mg-0 | Sample Mg-3 | Sample Mg-5 | Sample Mg-8 | Sample Mg-10 |
|---|---|---|---|---|---|
| Mg by WDS | 0 | – | 10.5 | 15.3 | 18.0 |

**Table S1 Mg composition estimated by WDS**

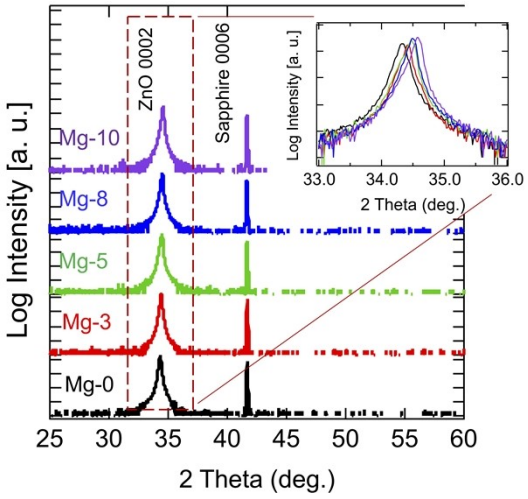


**Figure S1** XRD patterns of Mg-doped ZnO films with different nominal Mg compositions of 0 to 10 at%.

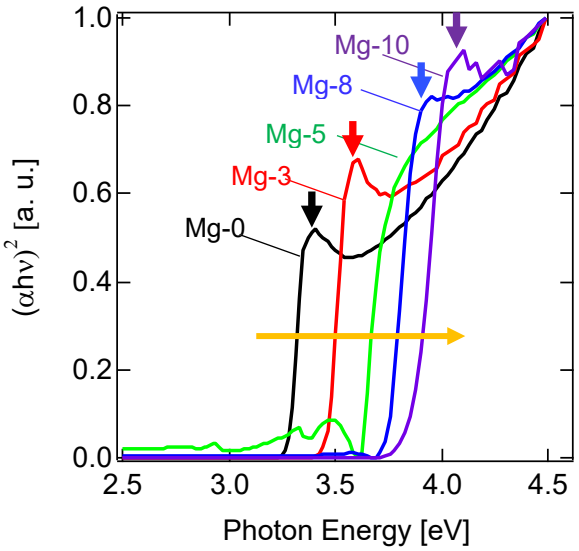

**Figure S2** Tauc plots from the optical absorption spectra of Mg-doped ZnO films with different nominal Mg compositions of 0 to10 at%. The arrows indicate the peak positions assigned to an excitonic absorption.

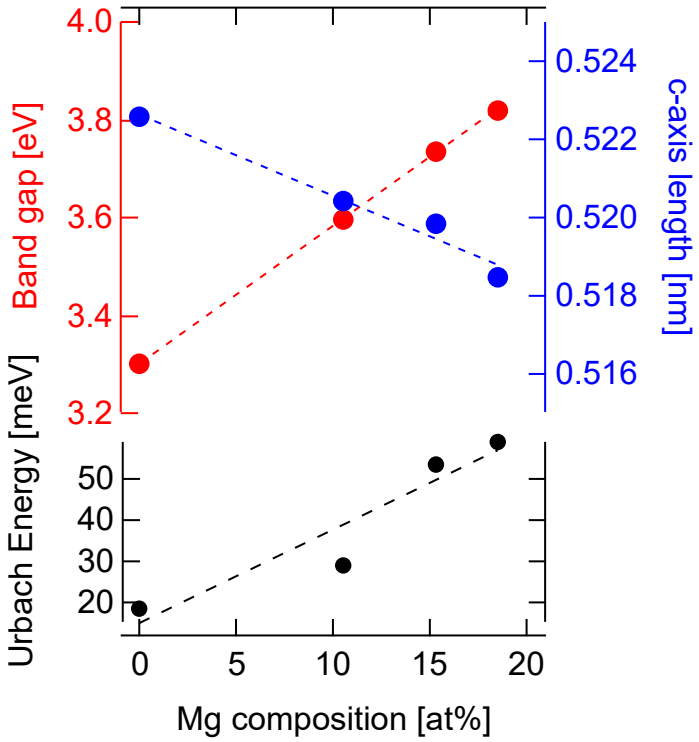


**Figure S3** Linear relationships of the band gap, the *c*-axis length and the Urbach energy to the Mg composition. Here, it should be noted that the data points for Sample Mg-3 were missing in the plots due to no WDS data of its Mg composition as listed in Table S1.

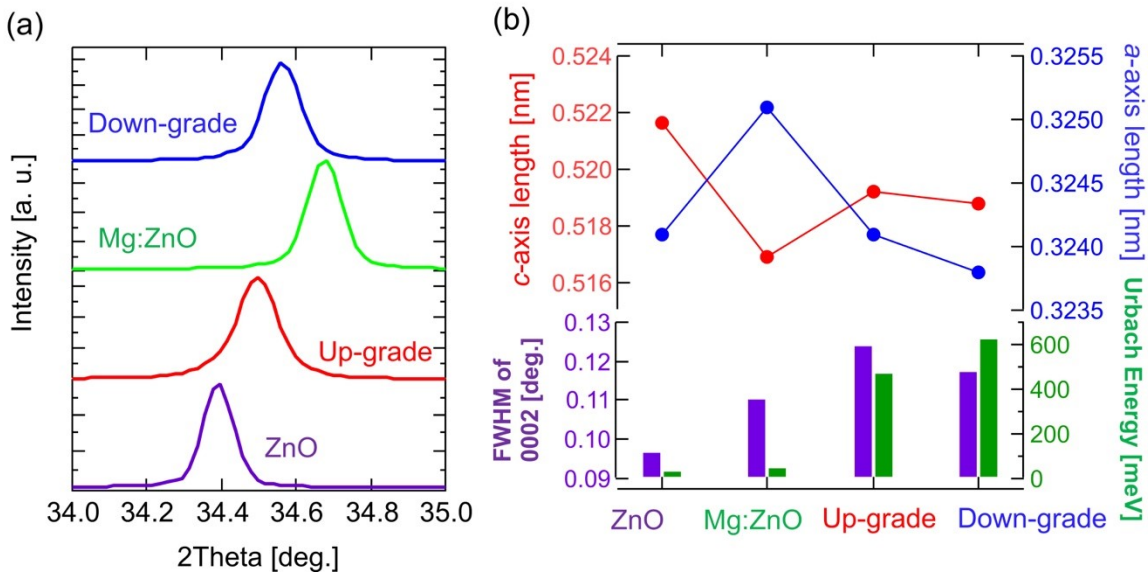


**Figure S4** For ZnO, Mg:ZnO, up-grade and down-grade Mg-ZnO films, (a) XRD patterns in linear scale intensity, (b) Plots of the *a*- and *c*-axis parameters, the FWHM values of the 0002 peak in the $\theta$-$2\theta$ scan, and the Urbach energy values.