

Supplementary Information

Morphology Effects in Photoactive ZnO Nanostructures: Photooxidative Activity of Polar Surfaces

Ana Iglesias-Juez,^{1,*} Francesc Viñes,² Oriol Lamiel-García,² Marcos Fernández-García,¹ and
Francesc Illas,^{2,*}

¹ Instituto de Catálisis y Petroleoquímica, CSIC, c/Marie Curie 2,
Cantoblanco, 28049 Madrid, Spain.

² Departament de Química Física & Institut de Química Teòrica i Computacional
(IQTCUB), Universitat de Barcelona, c/Martí i Franquès 1, 08028 Barcelona, Spain.

*corresponding authors: ana.iglesias@icp.csic.es, francesc.illas@ub.edu

Figure S1.- HR-TEM images and FFT diffraction patterns (from locations marked with a red colour box) for samples **A**, **B**, and **C**.

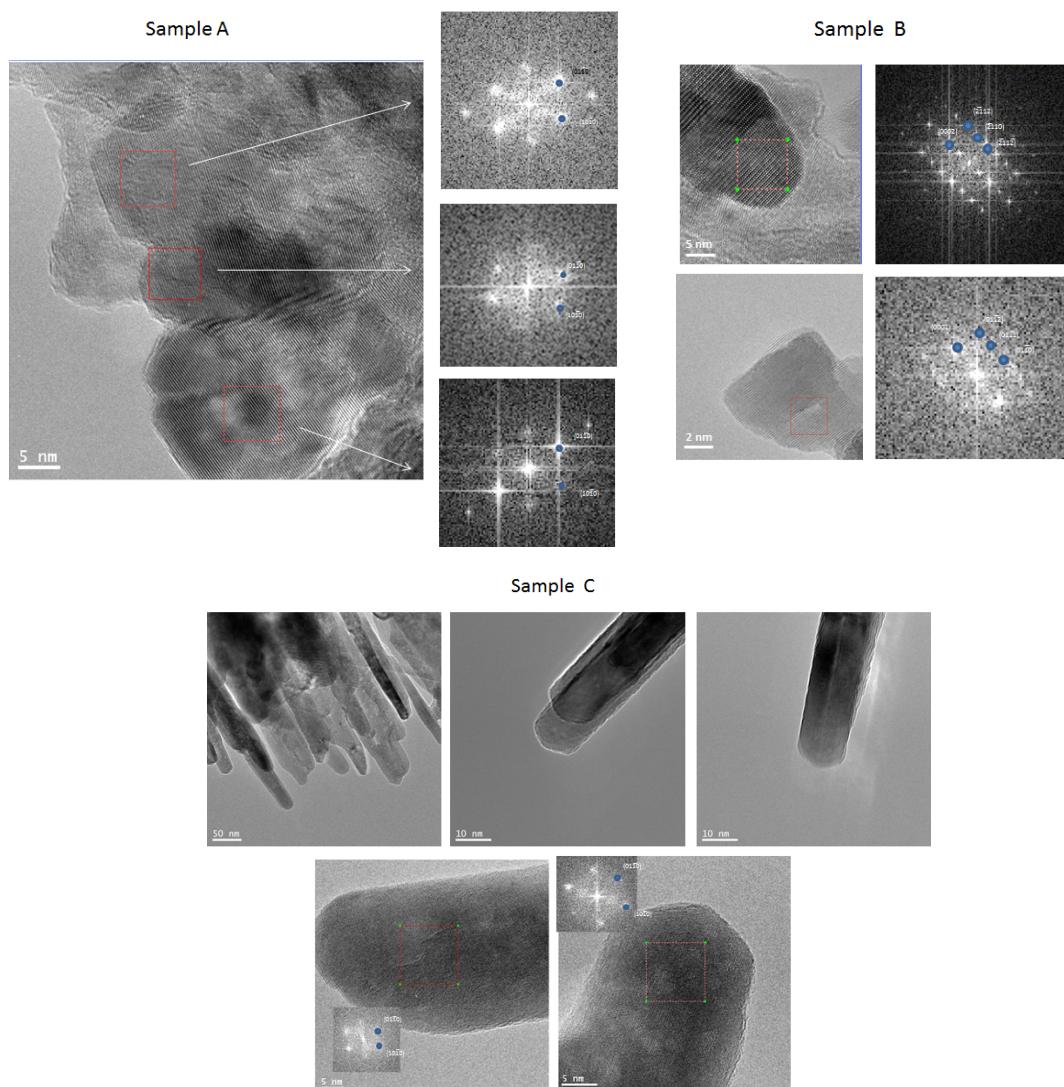


Figure S2.- Density of states of VB and CB of the pristine nonpolar $(10\bar{1}0)$ and $(11\bar{2}0)$ facets (green and blue), and of the polar (0001) and $(000\bar{1})$ planes (violet and red) with $\frac{1}{4}$ concentration of Zn and O vacancies, respectively.

