Electronic Supplementary Material (ESI) for Nanoscale.

Role of zinc interstitials and oxygen vacancies of ZnO in photocatalysis: A bottom-up approach to control the defect density

Fatma Kayaci, [a, b] Sesha Vempati, [a] * Inci Donmez, [a, b] Necmi Biyikli [a, b] and Tamer Uyar [a, b] *

[a] UNAM-National Nanotechnology Research Center, Bilkent University, Ankara, 06800, Turkey

[b] Institute of Materials Science & Nanotechnology, Bilkent University, Ankara, 06800, Turkey

Authors for correspondence: SV: svempati01@qub.ac.uk; TU: uyar@unam.bilkent.edu.tr

Supplementary Information

Figures:

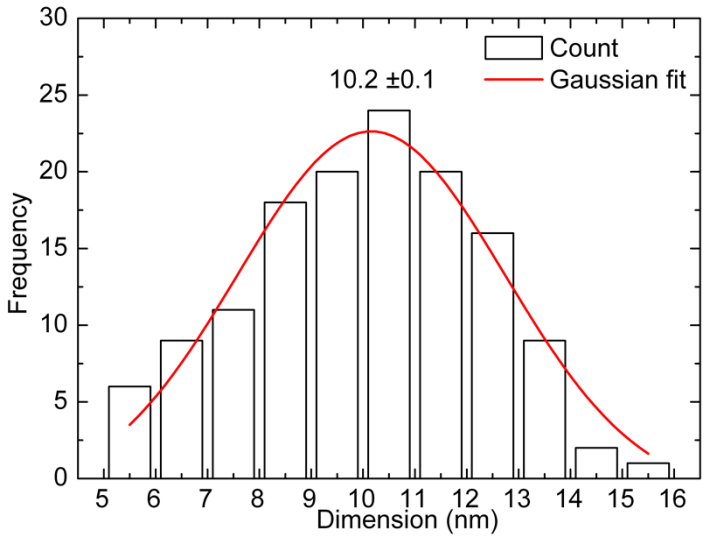

Figure S1. Particle size analysis from TEM image for PZ1 QD.

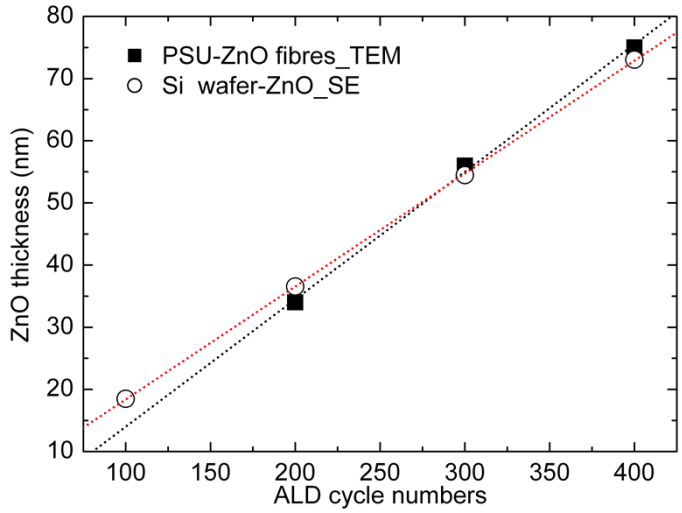

Figure S2. The thickness of ZnO as a function of ALD cycle numbers for two contexts, namely, PSU-ZnO fibers and ZnO coating on silicon wafer. The former case is from TEM image analysis, while the latter from spectroscopic ellipsometry (SE).

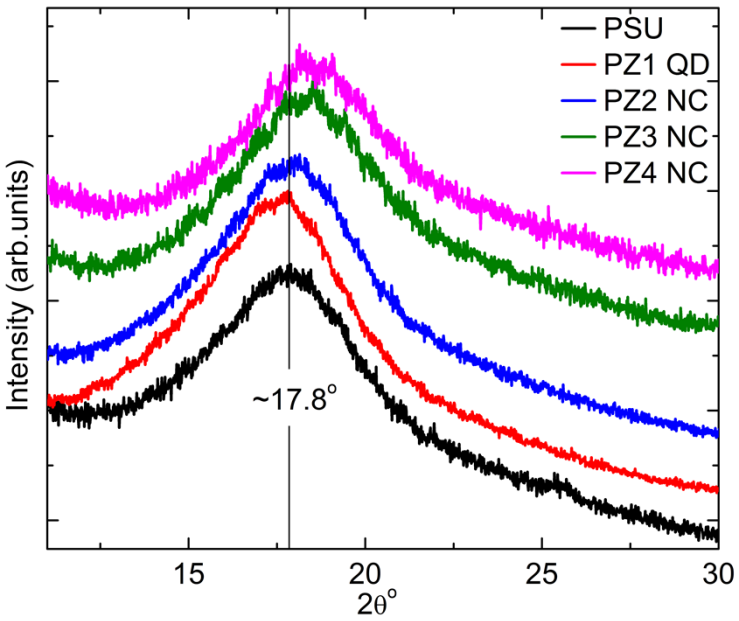

Figure S3. XRD patterns for pristine PSU and PSU-ZnO coated fibers within the region of ~10-30 .

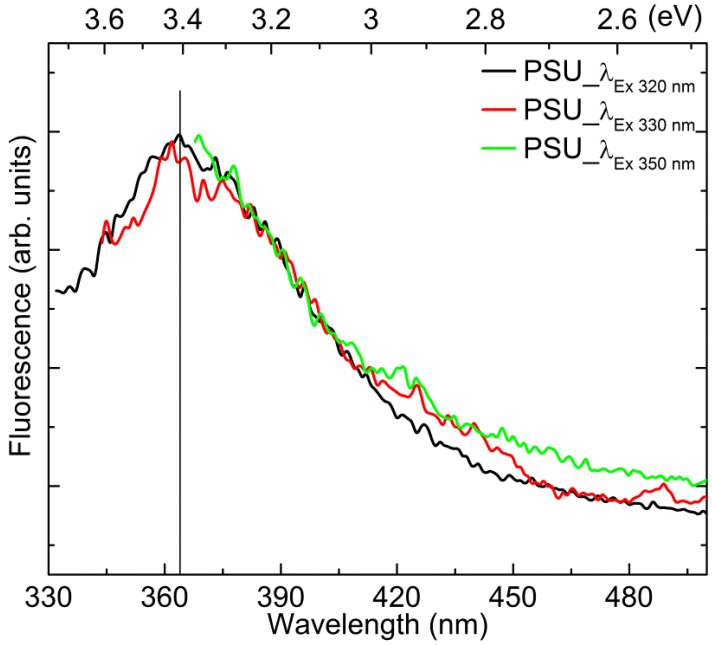

Figure S4. Emission spectra from pristine PSU electrospun fibers for three different excitations.

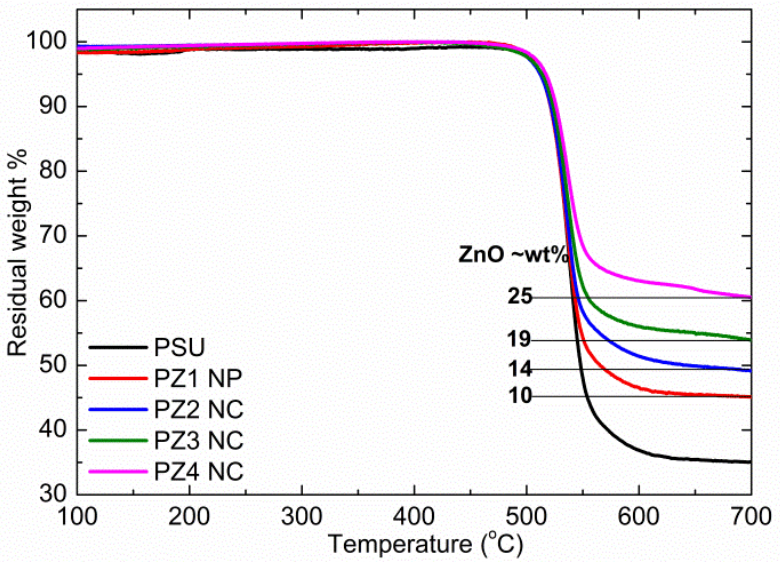

Figure S5. TGA of PSU-ZnO fiber samples compared with pristine PSU fibers.

Figure S5 Explanation: The derivative TGA thermograms (not shown here) of electrospun PSU and PSU-ZnO fibers is analyzed within the range of 450-625 °C. The decomposition of pristine PSU fibers occurred at ~538 °C, however after the ZnO coating, the peaks were shifted to ~536 °C. The reason for this slightly decreased thermal stability is might be due to the catalytic activity of ZnO causing early polymer decomposition [W. Li et al. J. Mater. Sci. 2009, vol 44, 2977; F. Kayaci et al., ACS Appl. Mater. Interfaces, 2012. vol 4, 6185-6194]

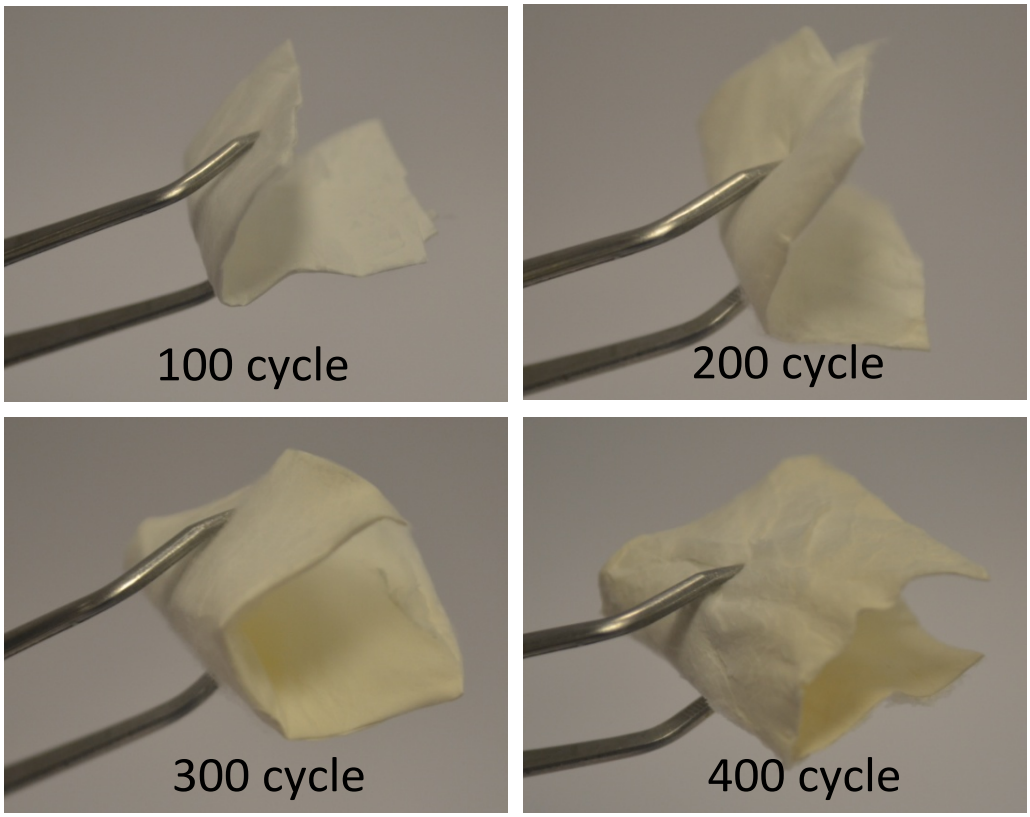

Figure S6. Digital photographs showing the convenience in handling the PSU-ZnO fibrous mats.

Tables:

Table S1. XRD characteristics of three selected peaks

Sample	(i)° **(100)**		(ii)° **(002)**		(iii)° **(101)**	
	FWHM	δ	FWHM	δ	FWHM	δ
PZ1 QD	1.239	-	1.055	-	1.135	-
PZ2 NC	1.150	**0.330**	0.983	**0.379**	0.957	**0.270**
PZ3 NC	0.680	**0.679**	0.646	**0.709**	0.713	**0.737**
PZ4 NC	0.759	**0.740**	0.667	**0.804**	0.751	**0.802**

Table S2. Output of peak fitting of photoluminescence showing error bar, where *fwhm*-full width at half of the maximum, *A*-area under the peak. L stands for Lorentzian shape while the rest of the peak shapes are Gaussian. The percentage increment in the defect density is calculated as follows.
For example, % increase for *b* emission = $b'= (A_{b \text{ from PZ1 QD}} - A_{b \text{ from PZ2, PZ3, PZ4 NC}})*100/ A_{b \text{ from PZ1 QD}}$

Sample	a_{1-4}		b_{1-4}		c_{1-4}		d_{1-4}		e_{1-4}	
	Peak position nm eV	*fwhm*/ *A* nm/ nm*counts	Peak position nm eV	*fwhm*/ *A* nm/ nm*counts	Peak position nm eV	*fwhm*/ *A* nm/ nm*counts	Peak position nm eV	*fwhm*/ *A* nm/ nm*counts	Peak position nm eV	*fwhm*/ *A* nm/ nm*counts
PZ1 QD	381.9 ± 0.3 3.25	17.5 ± 1.0 7.1 ± 1.8	399.5 ± 1.9 3.10	31.2 ± 3.2 17.5 ± 4.4	433.2 ± 1.6 2.86	63.9 ± 1.9 66.9 ± 3.4	501.2 ± 1.9 2.47	56.4 ± 1.3 12.5 ± 0.3	565.6 ± 15.5 2.19	82.4 ± 3.4 5.4 ± 0.2
PZ2 NC	385.8 ± 0.2 3.21	24.9 ± 1.3 14.9 ± 4.8	404.5 ± 4.2 3.06	38.5 ± 6.8 22.7 ± 13.9	431.8 ± 7.8 2.87	61.9 ± 5.6 34.6 ± 9.6	498.4 ± 2.5 2.49	67.9 ± 1.1 13.7 ± 0.2	564.8 ± 12.5 2.20	102.7 ± 1.4 9.83 ± 0.1
PZ3 NC	389.7 ± 0.3 3.18	21.7 ± 1.3 12.5 ± 4.3	407.1 ± 3.6 3.04	34.2 ± 5.0 21.4 ± 9.0	435.7 ± 7.5 2.85	63.0 ± 3.9 33.1 ± 6.1	498.7 ± 2.0 2.49	74.1 ± 6.5 59.9 ± 15.5	561.8±18.3 2.21	98.2 ± 12.2 23.0 ± 9.6
PZ4 NC	388.7 ± 0.2 3.19	21.2 ± 1.09 12.3 ± 3.4	406.6 ± 2.7 3.04	34.5 ± 4.2 23.4 ± 8.1	437.2 ± 6.8 2.83	63.1 ± 4.8 32.8 ± 6.5	499.9 ± 2.0 2.48	73.1 ± 6.4 52.2 ± 12.2	565.9 ± 17.7 2.19	95.3 ± 12.2 18.2 ± 7.5

	P′(L)		*P″*	
Sample	Peak position nm eV	*fwhm*/ *A* nm/ nm*counts	Peak position nm eV	*fwhm*/ *A* nm/ nm*counts
PSU	365.4 ± 0.2	79.3 ± 0.9 0.84 ± 0.0	-	-
PZ1 QD	-	-	364 ± 1.8	25.5 ± 2.5 10.9 ± 2.8