Tuning Surface Oxygen Concentration of {111} Surrounded Ceria Nanocrystals for Enhanced Photocatalytic Activity

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Supporting Information

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Table-1:

Indium doping concentration (wt. %)	2-Theta	Lattice parameter(nm)	d-spacing (nm)	Crystalline size (nm)
0	28.287	0.541	0.3146	5.812
5	28.344	0.537	0.312	5.295
10	28.362	0.529	0.309	5.142
15	28.415	0.520	0.307	5.061

The calculated crystallite size by Scherrer formula in equation (1) decreased with increasing the indium content with the size was about 5–6 nm.

$$D = k\lambda/\beta\cos\theta \quad (1)$$

In this equation1, k is a constant equal to 0.89, λ is the X-ray wavelength equal to 0.154 nm, β is the full width at half maximum, and θ is the half diffraction angle.

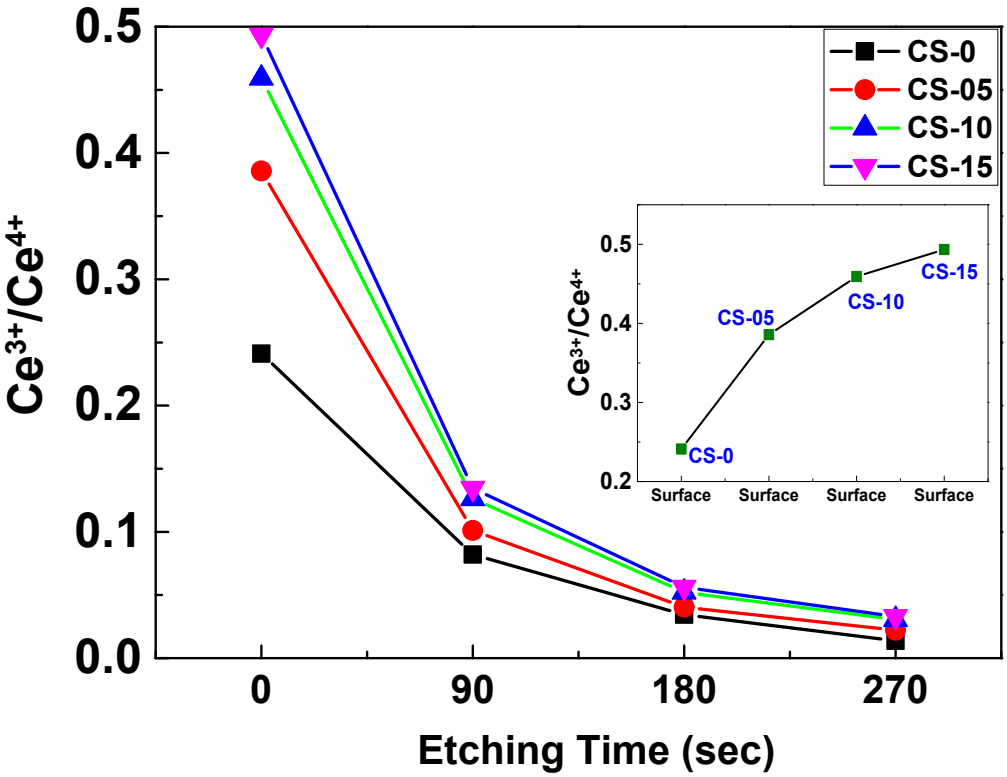

Figure S1: Variations in Ce^{3+}/Ce^{4+} ratios of un doped and doped CeO_2 extracted from XPS data with respect to etching time by using 3keV Ar ion beam

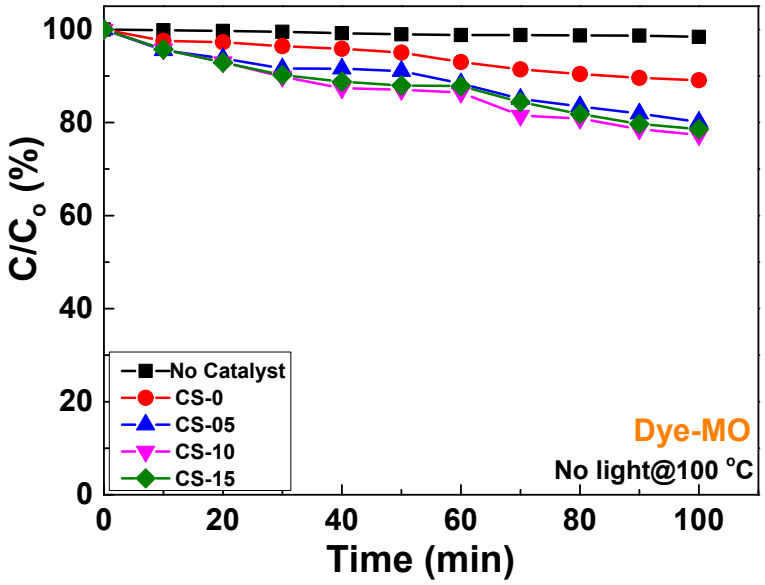

Figure S2: Thermocatalytic performances of all samples (doped and undoped CeO_2 nanocrystals) under dark conditions.

The rate constant at room temperature is denoted as κ_p, while the rate constants for thermocatalytic reactions(only at high temperature without any radiation) and photothermocatalytic reactions(with visible and UV light radiations and at high temperatures are denoted as κ_t and κ_{tp}, respectively as shown in figure S3.

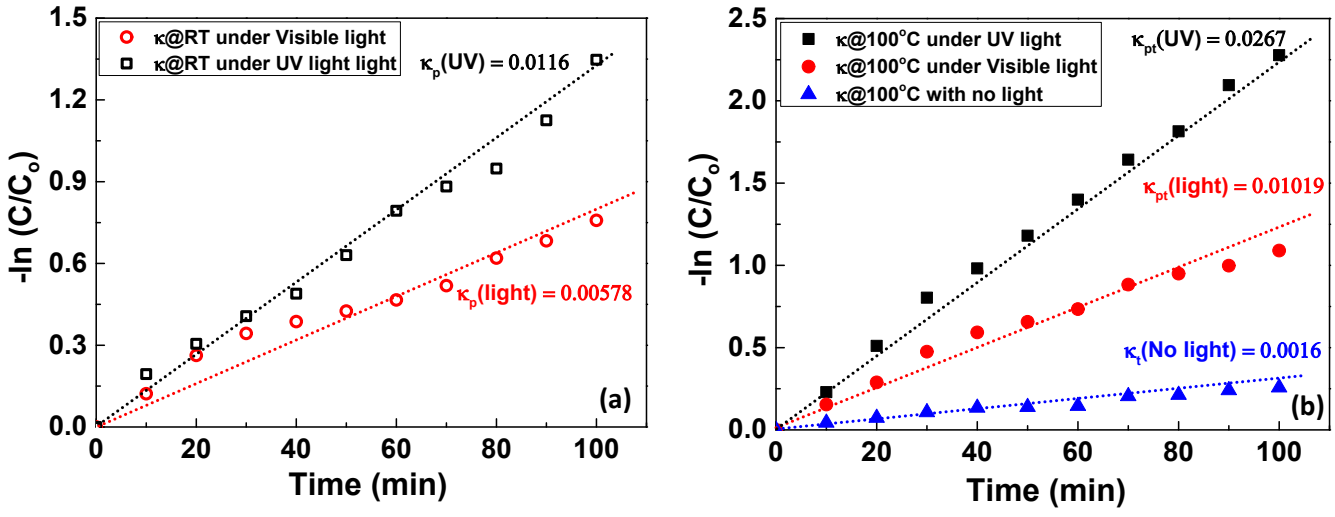

Figure S3: Plot of rate constants for Photocatalytic Degradation of MO (a) at Room Temperature (b) Thermocatalytic Degradation at 100 °C, and Photo-thermocatalytic Degradation at 100 °C of CS-10 sample.

If the photo-thermocatalytic reaction is assumed to be due to the photocatalytic degradation in parallel with the thermocatalytic degradation that proceeds independently, then, the rate of dye decolourization would be equal to the sum of κ_t and κ_p. However, by analysing rate constant results carefully, the κ_{tp} under UV light radiation and visible light radiation are almost 2.1 and 1.7 times higher than the sum of κ_t and κ_p. This further confirms the efficient electron hole separation at elevated temperatures due to the mobility of oxygen ions leading to a synergistic effect for the dye degradation.

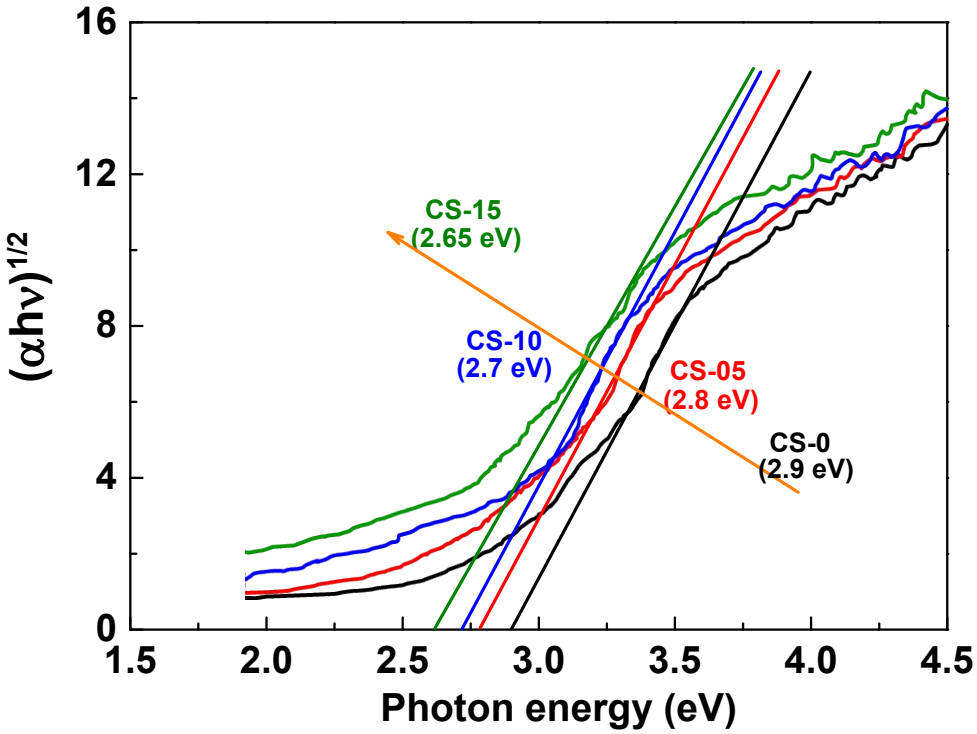

Figure S4: Schuster-Kubelka-Munk absorption function of In–doped CeO_2 samples with x-intercept showing the band gap energies.