Supporting Information for

Design, synthesis, and characterization of CeO_2 and SnO_2 nanoparticles for enhanced UVA-light-driven photocatalysis

$$\boldsymbol{E_g = E_{LUMO} - E_{HOMO}} \quad \textbf{(1)}$$

$$\boldsymbol{\mu = \frac{1}{2}(E_{LUMO} + E_{HOMO})} \quad \textbf{(2)}$$

$$\boldsymbol{\eta = \frac{1}{2}(E_{LUMO} - E_{HOMO})} \quad \textbf{(3)}$$

$$\boldsymbol{\omega = \frac{\mu^2}{2\eta}} \quad \textbf{(4)}$$

Where E_{HOMO}, E_{LUMO} Eg, η, μ and ω are the energy of the highest occupied molecular orbital, the energy of the lowest unoccupied molecular orbital, the frontier orbital gap, the chemical hardness, the electronic chemical potential and the electrophilicity (ω) of materials.

$$\boldsymbol{E_{h\nu\ or\ g} = \frac{1240}{\lambda}} \quad \textbf{(5)}$$

where λ is the excitation wavelengths of UVA-light irradiation lamp of the photoreactor or that corresponding to the absorption band of material.

$$\eta(\%) = [\frac{(C_i - C_{60})}{C_i}]\,100 \quad \textbf{(6)}$$

$$\eta'(\%) = [\frac{(C_{60} - C_f)}{C_{60}}]\,100 \quad \textbf{(7)}$$

where C_i : dye initial concentration ($mg\cdot L^{-1}$). C_{60} : dye residual concentration after adsorption/desorption equilibrium ($mg\cdot L^{-1}$) and C_f : dye residual concentration under oxidation conditions after certain intervals (mgL^{-1}).

$$\boldsymbol{n\lambda = d_{hkl} 2 \sin\theta_{hkl}} \quad (8)$$

where n, λ, d_{hkl} and θ_{hkl} denote the diffraction order (usually n = 1), X-ray wavelength (nm), Bragg diffraction angle (degree) and d-spacing (Å), respectively.

$$\mathbf{d_{hkl}} = \frac{\mathbf{a}}{\sqrt{\mathbf{h^2 + k^2 + l^2}}} \quad (9)$$

$$\frac{\mathbf{1}}{\mathbf{d_{hkl}}} = \sqrt{\frac{\mathbf{h^2 + k^2}}{\mathbf{a^2}} + \frac{\mathbf{l}}{\mathbf{c^2}}} \quad (10)$$

$$\boldsymbol{V = a^3} \quad (11)$$

$$\boldsymbol{V = a^2 c} \quad (12)$$

$$\mathbf{d} = \sum \frac{\mathbf{A}}{\boldsymbol{N_A}\mathbf{V}} \quad (13)$$

Where A is the sum of atomic weight of all the atoms of the unit cell, N_A is the Avogadro's number (6.0221×10^{23} mol^{-1}).

$$d_{CeO2} = \sum \frac{4\,M_{CeO2}}{\mathrm{N}\,a^3} \quad (14)$$

$$d_{SnO2} = \sum \frac{2\,M_{SnO2}}{\mathrm{N\,V}} \quad (15)$$

Here, M_{CeO2} and M_{SnO2} are the molecular weights of the particular CeO_2 (172.115 g.mol^{-1}) SnO_2 (M=150.71 g.mol^{-1}).

$$\varepsilon = \frac{\beta_{hkl}}{4\tan\theta_{hkl}} \quad (16\ )$$

$$\delta = \frac{1}{(\mathrm{D_{XRD}})^2} \quad (17)$$

$$\mathrm{SSA} = \frac{6000}{\rho \mathrm{D_{XRD}}} \quad (18)$$

where D_{XRD} is the average particle size (nm) and ρ is the theoretical density of CeO_2-500 and SnO_2-450 (g.cm^{-3}).

$$\mathrm{n} = \frac{\pi(D_{XRD})^3}{6\mathrm{V}} \quad (19)$$

$$\beta_{hkl}^2 = \beta_m^2 - \beta_i^2 \quad (20)$$

β_m and β_i values of the explored materials were estimated through the full-width at half maxima (FWHM=β_{hkl}).

$$D_{XRD} = \frac{K\lambda}{\beta_{hkl}\cos\theta_{hkl}} \quad (21)$$

where D_{XRD} is the average crystallite size (nm), K is the shape constant (K =0.89 for cubic crystal struture), λ is the wavelength of the Cu-radiation (λ =0.15406 nm for $CuK_{\alpha 1}$), β_{hkl} is FWHM of the peak (radians), and θ_{hkl} is the diffraction angle (degree).

$$\cos\theta_{hkl} = \frac{k\lambda}{D_{XRD}}\left(\frac{1}{\beta_{hkl}}\right) \quad (22)$$

$$\mathrm{Slope} = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2} \quad (23)$$

$$\beta_{hkl} = \frac{k\lambda}{D_{XRD}}\left(\frac{1}{\cos\theta_{hkl}}\right) \quad (24)$$

$$\ln\beta_{hkl} = \ln\left(\frac{k\lambda}{D_{XRD}}\right) + \ln\left(\frac{1}{\cos\theta_{hkl}}\right) \quad (25)$$

$$\ln\left(\frac{k\lambda}{D_{XRD}}\right) = Intercept \quad (26)$$

$$\frac{k\lambda}{D_{XRD}} = e^{(Intercept\omega t)} \quad (27)$$

$$\beta_{hkl} = \beta_{size} + \beta_{strain} \quad (28)$$

$$\beta_{strain} = 4\varepsilon\ \tan\theta_{hkl} \quad (29)$$

$$\beta_{size} = \frac{k\lambda}{D_{XRD}\cos\theta_{hkl}} \quad (30)$$

$$\beta_{hkl} = \frac{k\lambda}{D_{XRD}\cos\theta_{hkl}} + 4\varepsilon\ \tan\theta_{hkl} \quad (31)$$

where ε is the intrinsic strain in the crystal lattice.

$$\beta_{hkl} \cos\theta_{hkl} = \frac{k\lambda}{D_{XRD}} + 4\varepsilon(\sin\theta_{hkl}) \quad (32)$$

$$y = mx + c \quad (33)$$

$$\sigma = Y_{hkl}\varepsilon \quad (34)$$

where Y_{hkl} is Young's modulus.

$$\beta_{hkl} \cos\theta_{hkl} = \frac{k\lambda}{D_{XRD}} + \left(\frac{\sigma}{Y_{hkl}}\right) 4 \sin\theta_{hkl} \quad (35)$$

$$\frac{1}{Y_{hkl}} = S_{11} - 2(S_{11} - S_{12} - 0.5(S_{44})\left[\frac{h^2k^2 + k^2l^2 + h^2l^2}{(h^2 + k^2 + l^2)^2}\right] \quad (36)$$

$$S_{11} = \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \quad (37)$$

$$S_{12} = \frac{-C_{11}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \quad (38)$$

$$S_{44} = \frac{1}{C_{44}} \quad (39)$$

$$\frac{1}{Y_{hkl}} = \frac{S_{11}(h^4 + k^4) + (2S_{11} + S_{66})h^2k^2 + 2(S_{13} + S_{44})(h^2 + k^2)l^2 + S_{33}l^4}{(h^2 + k^2 + l^2)^2} \quad (40)$$

Where h, k and l are Miller indexes of the crystallographic plane.

$$S_{11} = \frac{C_{33}}{2C} + \frac{1}{2(C_{11} - C_{12})} \quad (41)$$

$$S_{12} = \frac{C_{33}}{2C} - \frac{1}{2(C_{11} - C_{12})} \quad (42)$$

$$S_{13} = -\frac{C_{13}}{C} \quad (43)$$

$$S_{33} = \frac{(C_{11} + C_{12})}{C} \quad (44)$$

$$S_{44} = \frac{1}{C_{44}} \quad (45)$$

$$S_{66} = \frac{1}{C_{66}} \quad (46)$$

$$C = (C_{11} + C_{12})C_{33} - 2C_{13}^2 \quad (47)$$

$$u = \varepsilon^2\left(\frac{Y_{hkl}}{2}\right) \quad (48)$$

$$u = \frac{\sigma^2}{2Y_{hkl}} \quad (49)$$

$$\varepsilon = \sigma\sqrt{\frac{2u}{Y_{hkl}}} \quad (50)$$

$$\beta_{hkl} \cos\theta_{hkl} = \frac{k\lambda}{D_{XRD}} + 4 \sin\theta_{hkl}\left(\frac{2u}{Y_{hkl}}\right)^{1/2} \quad (51)$$

$$\beta_{hkl} = \beta_L + \beta_G \quad (52)$$

$$(d_{hkl}\beta_{hkl} \cos\theta_{hkl})^2 = \frac{k\lambda}{D_{XRD}}\,({d_{hkl}}^2\beta_{hkl} \cos\theta_{hkl}) + \left(\frac{\varepsilon}{2}\right)^2 \quad (53)$$

$$(d_{hkl}\beta_{hkl}\cos\theta_{hkl})^2 = \frac{k\lambda}{D_{XRD}}\,(d_{hkl}{}^2\beta_{hkl}\cos\theta_{hkl}) + \left(\frac{\varepsilon\lambda}{2}\right)^2 \quad (54)$$

$$\beta_{hkl}^2 = \beta_L\,\beta_{hkl} + \beta_G^2 \quad (55)$$

Where β_L and β_G stands are the full width at half maximum of the Lorentzian and Gaussian function.

$$\left(\frac{\beta_{hkl}^*}{d_{hkl}^*}\right)^2 = \frac{1}{D_{XRD}}\left(\frac{\beta_{hkl}^*}{d_{hkl}^*{}^2}\right) + \left(\frac{\varepsilon}{2}\right)^2 \quad (56)$$

$$\beta_{hkl}^* = \beta_{hkl}\frac{\cos\theta_{hkl}}{\lambda} \quad (57)$$

$$d_{hkl}^* = 2d_{hkl}\frac{\sin\theta_{hkl}}{\lambda} \quad (58)$$

$$\left(\frac{\beta_{hkl}}{\tan\theta_{hkl}}\right)^2 = \frac{k\lambda}{D_{XRD}}\left(\frac{\beta_{hkl}\cos\theta_{hkl}}{\sin^2\theta_{hkl}}\right) + 16\varepsilon^2 \quad (59)$$