Exploring the Facet-engineered Anatase Nanoparticles for amplification of Sensitivity in Heavy Metal Ion Detection and Other Applications

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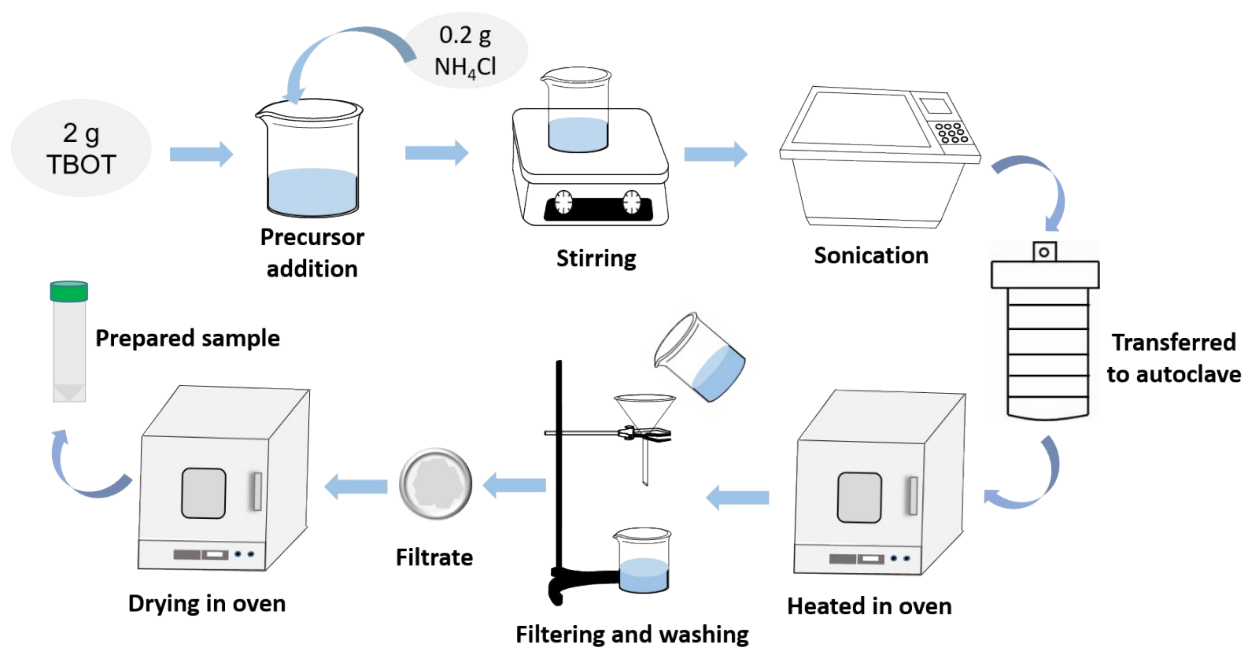
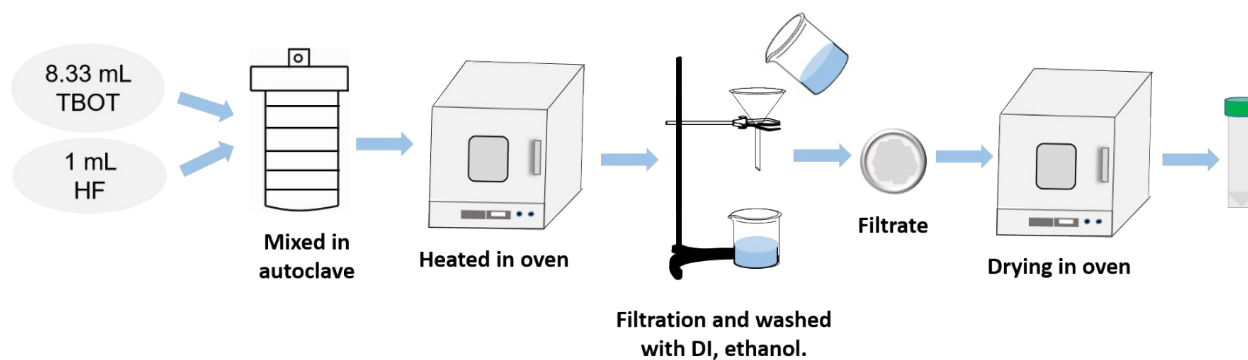**Figure S1: Schematic depiction of the synthesis procedure of {101}-faceted TiO₂.**

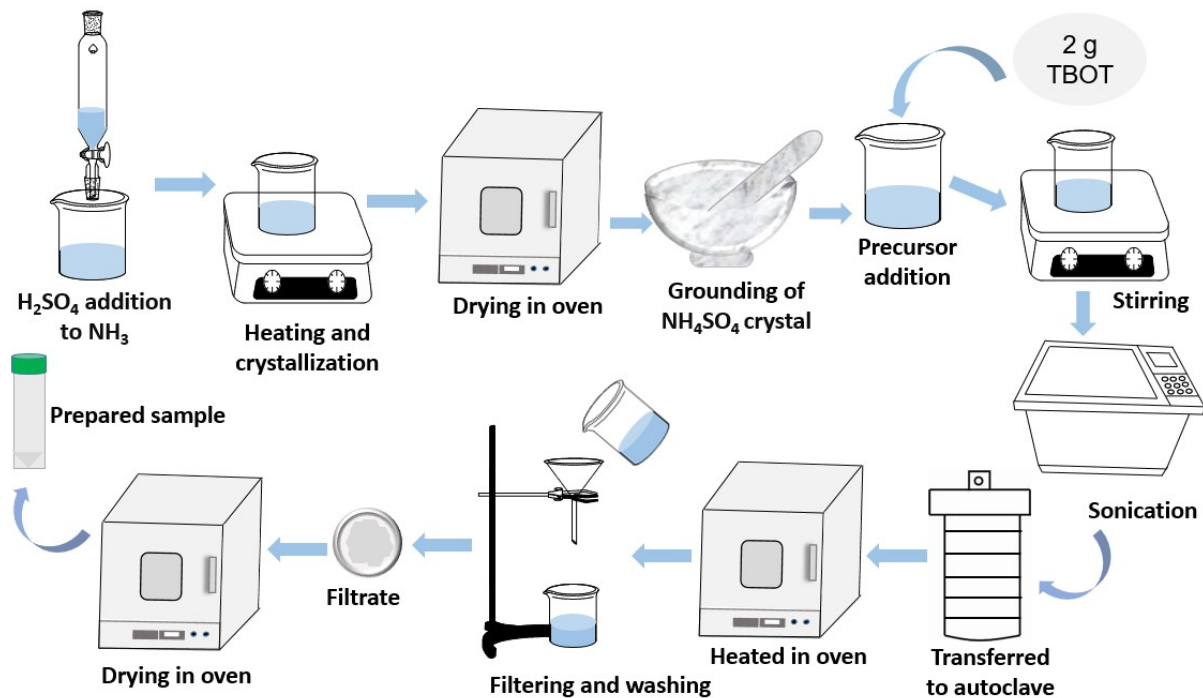**Figure S2: Schematic depiction of the synthesis procedure of {001}-faceted TiO₂.**

Figure S3: Schematic depiction of the synthesis procedure of {101}/{001 co--faceted TiO$_2$.

Lattice parameter, $\frac{1}{(d_{hkl})^2} = \left(\frac{h^2 + k^2}{a^2}\right) + \frac{l^2}{c^2}$ (E1)

Crystallite size, $D = \frac{K\lambda}{\beta cos\theta}$ (E2)

Dislocation density $, \delta = \frac{1}{(\text{Crystallite size})2}$ (E3)

Microstrain $, \in = \frac{FWHM}{4\tan(\Theta)}$ (E4)

Crystallinity index $= \frac{H(004) + H(200) + H(105)}{H(101)}$

(E5)

Here, D = size of crystallite; K = 0.9 = shape factor; h, k, and l = planes of the unit cell; λ = wavelength, θ = diffraction angle (degree), d_{hkl} = interplanar distance, β (in radian) = FWHM = full width at half maximum; H = height of the correlating plane's peak.

$$\text{Relative intensity} = \frac{I_{(101)}}{I_{(004)} + I_{(200)} + I_{(105)}}$$

(E6)

$$\text{Preference growth} = \frac{Relative\ intensity_{sample} - Relative\ intensity_{standard}}{Relative\ intensity_{standard}}$$

(E7)

$$\text{Texture coefficient, } T_C = \frac{I/I_o}{N^{-`1}} \left(\sum_n I/I_o \right)^{-1}$$

(E8)

In this context, N represents the number of reflections, I_o signifies the average intensity of the plane as obtained from the JCPDS data, and I refers to the relative intensity of a specific plane as observed.
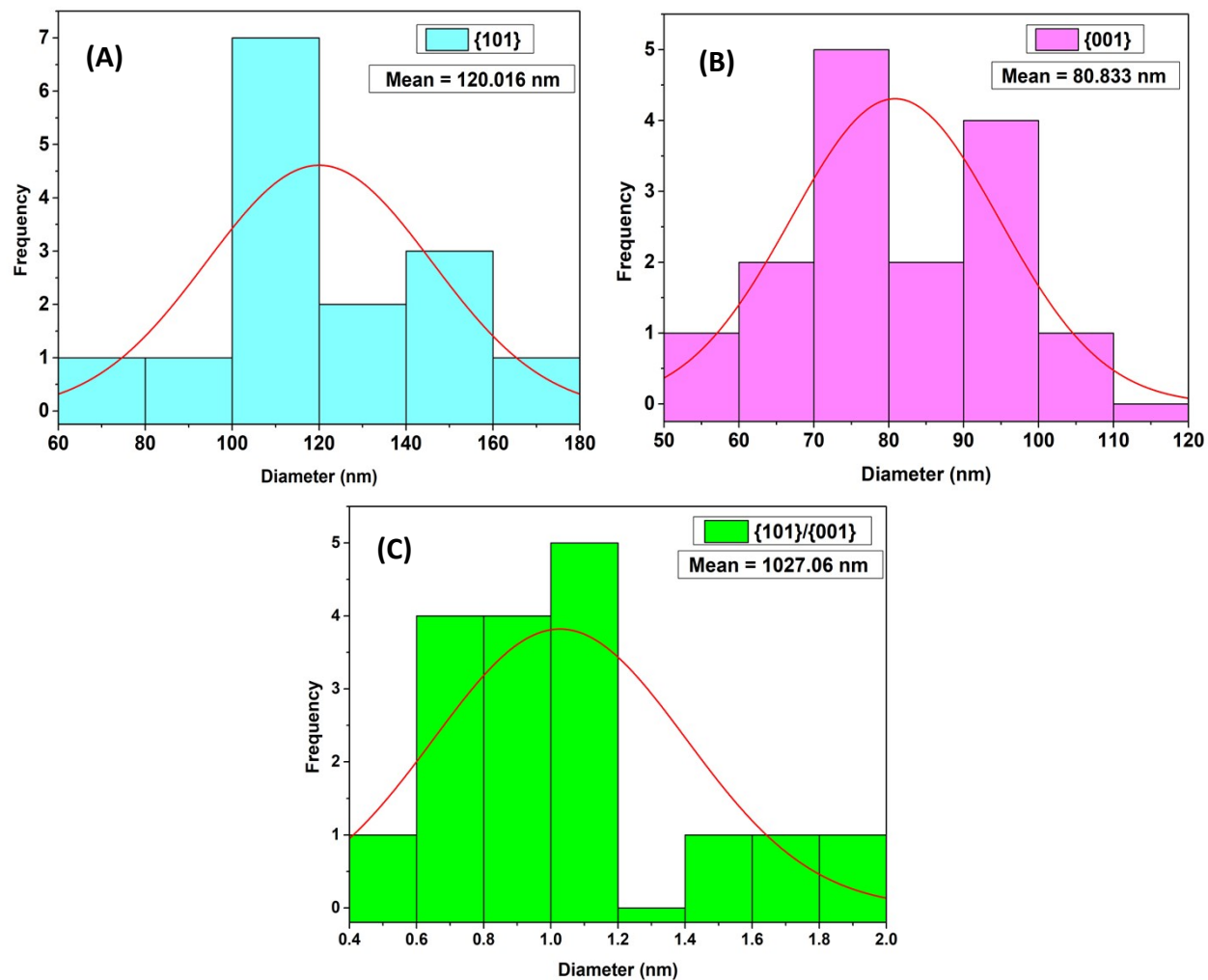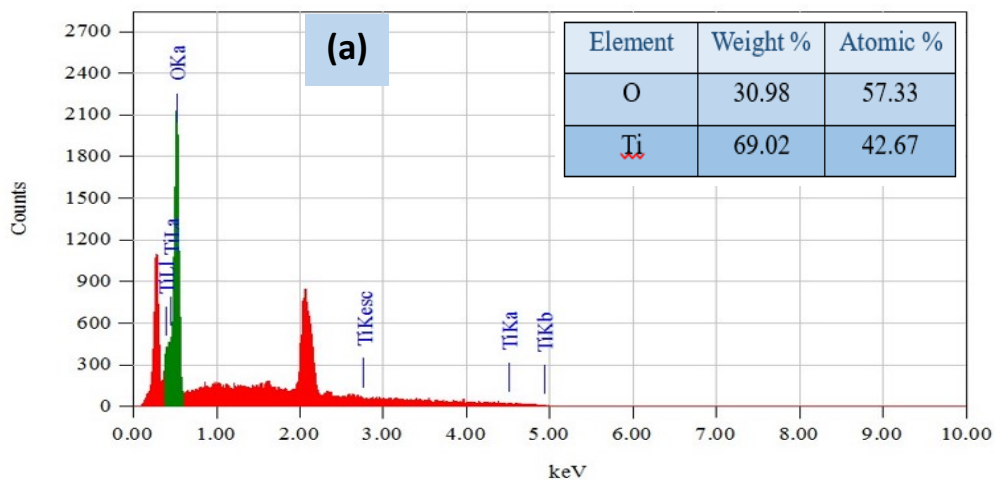
Figure S4: Histogram analysis of the synthesized {101}-faceted, {001}-faceted and {101/{001} co-faceted TiO₂ samples.
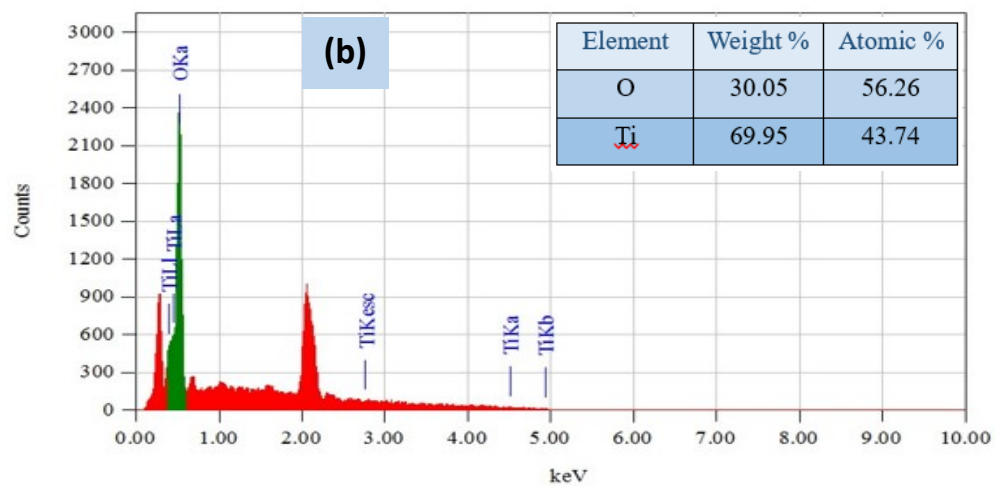

Element	Weight %	Atomic %
O	30.98	57.33
Ti	69.02	42.67

Figure S5: EDX spectra with elemental mapping of the synthesized (a) {101}-faceted (b) {001}-faceted TiO$_2$ samples