Water-induced stacking α-Fe_2O_3 hexagonal nanoplates along the [001} direction and its facet-dependent catalytic performances

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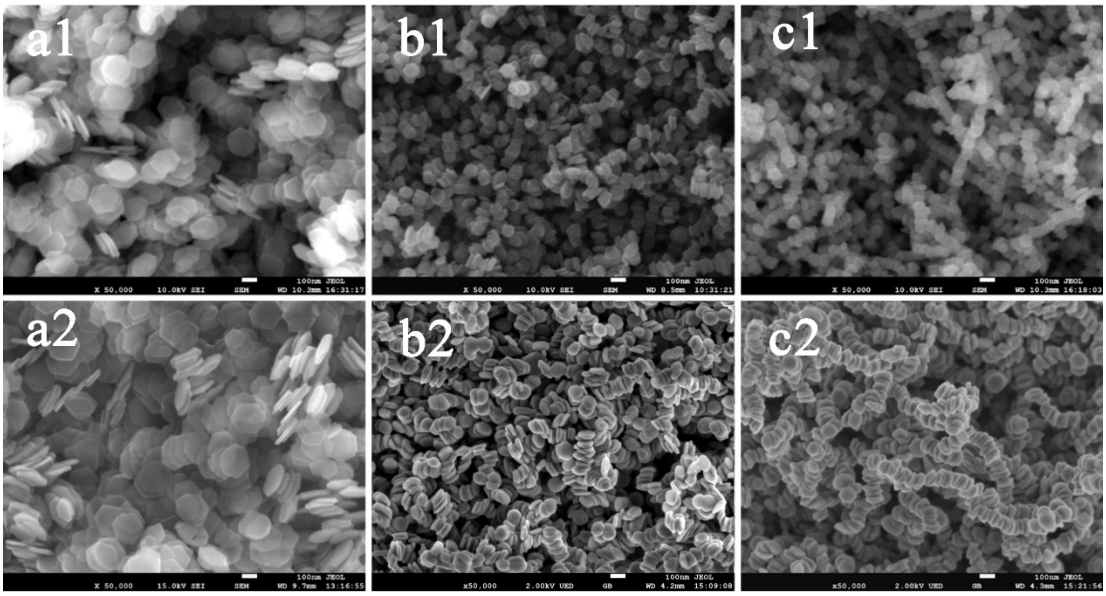

Fig. S1 SEM images of α-Fe_2O_3 nanoparticles: (a1, a2) α-Fe_2O_3 HNP, (b1, b2) α-Fe_2O_3 SSHNP and (c1, c2) α-Fe_2O_3 LSHNP.

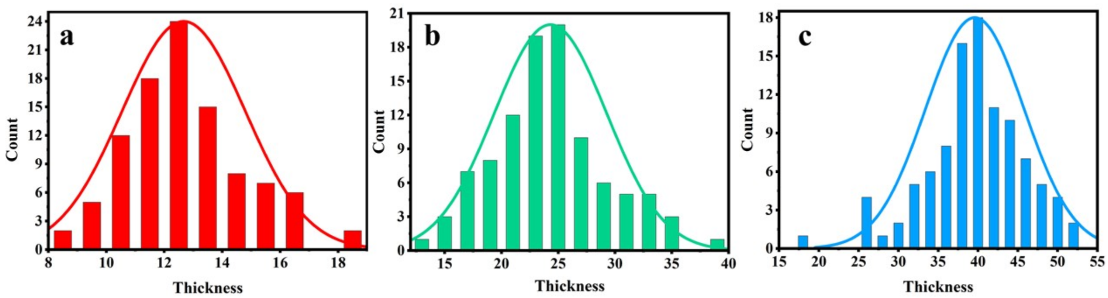

Fig. S2 The statistical graph of HNP thickness for α-Fe_2O_3 (a) HNP, (b) SSHNP and (c) LSHNP.

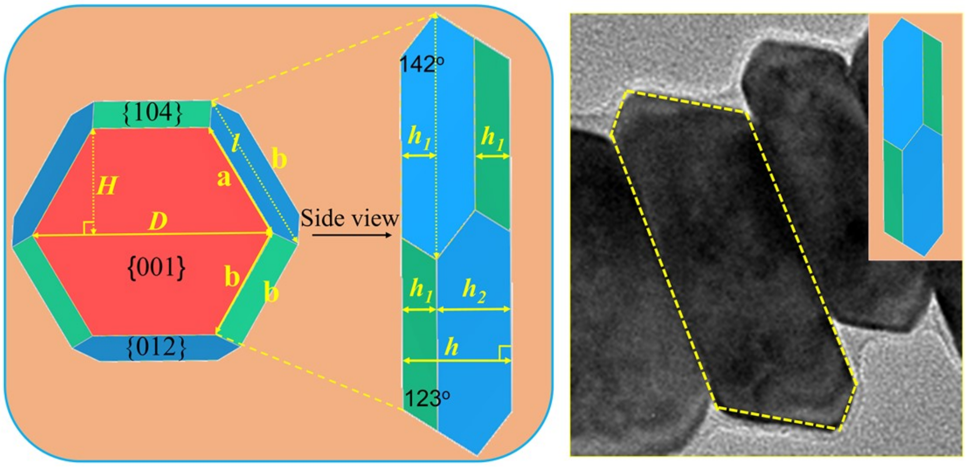

Fig. S3 The ideal crystal model of HNP for α-Fe_2O_3.

In fact, the thickness and diameter of nanoplate in the same sample are uneven, especially in SSHNP and LSHNP. Moreover, the stacked structures do not completely cover the {001} facets, therefore it is difficult to achieve an accurate quantification. Herein, we used an ideal model and average parameters to obtain the ratios of facets to reflect the increase trend of {012}+{104}, thus calculation method in this work is semi-quantitative, and the specific calculation process is as follows:

$$S_{001} = 2 \times \left[\frac{1}{2} \times (a + D) \times H + \frac{1}{2} \times (b + D) \times H\right]$$

$$S_{104} = 6 \times b \times \frac{h_1}{cos(142^{\circ} - 90^{\circ})}$$

$$S_{012} = 6 \times \left[\frac{1}{2} \times (a + l) \times \frac{h_1}{cos(123^{\circ} - 90^{\circ})} + \frac{1}{2} \times (b + l) \times \frac{h_2 - h_1}{cos(123^{\circ} - 90^{\circ})}\right]$$

$$l = \frac{\frac{h_1}{tan(180° - 142°)} + \frac{h_2 - h_1}{tan(180° - 123°)} + a \times cos(\Theta)}{cos(\Theta)}$$

Where ***D*** is the average diameter of hexagonal nanoplates; ***a*** and ***b*** are the side length of {012} and {104}, respectively; ***H*** is the height of trapezium section in hexagonal {001} plane; ***l*** is diagonal of {012} which links the two {104} facets; ***h*** is the thickness of nanoplate; h_1 and h_2 is the thickness of {012} and {104} in side view, respectively. Θ is the angle between ***a*** and the vertical normal line.

After measured we found that the side length of hexagon was nearly the same, so we made ***a*** equals to ***b***, therefore we can conducted the conclusions as follows:

$D = 2a; H = a \times \cos(30^\circ); h_1 = h_2 - h_1; h = 3h_1; \Theta = 30^\circ$

$$S_{001} = 3\sqrt{3}a^2$$

$$S_{104} = \frac{2ah}{cos(52^\circ)}$$

$$S_{012} = \frac{2h(a+l)}{cos(33^\circ)}$$

$$l = \frac{h}{3tan(38^\circ)cos(30^\circ)} + \frac{h}{3tan(57^\circ)cos(30^\circ)} + a$$

$$R_{HNP} = \frac{S_{012} + S_{104}}{S_{001}}$$

$$R_{SSHNP} = 6 \times \frac{S_{012} + S_{104}}{S_{001}}$$

$$R_{LSHNP} = 18 \times \frac{S_{012} + S_{104}}{S_{001}}$$

Tab. S1 The side length and thickness statistics and facet ratios of three samples.

Sample	Side length (*a*) (nm)	Thickness (*h*) (*nm*)	Ratio of surface area {012}+{104}/ {001}
α-Fe_2O_3 HNP	65	12	0.296
α-Fe_2O_3 SSHNP	45	25	5.775
α-Fe_2O_3 LSHNP	35	40	39.756

a and h are the average values of statistics.

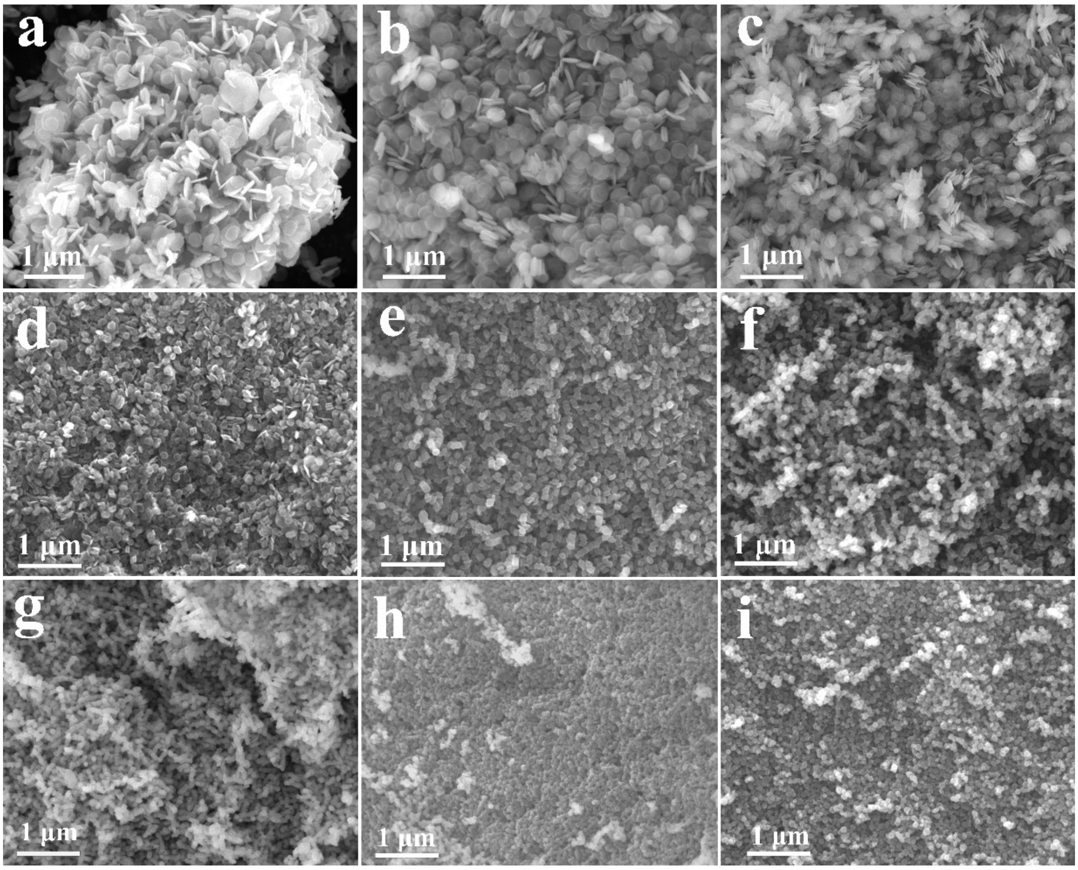

Fig. S4 SEM images in low magnification of α-Fe_2O_3 nanoplates with different H_2O content. (a) 0 mmol, (b) 28 mmol, (c) 56 mmol-HNP, (d) 111 mmol, (e) 222 mmol-SSHNP, (f) 333 mmol, (g) 444 mmol-LSHNP, (h) 555 mmol, (i) 666 mmol.

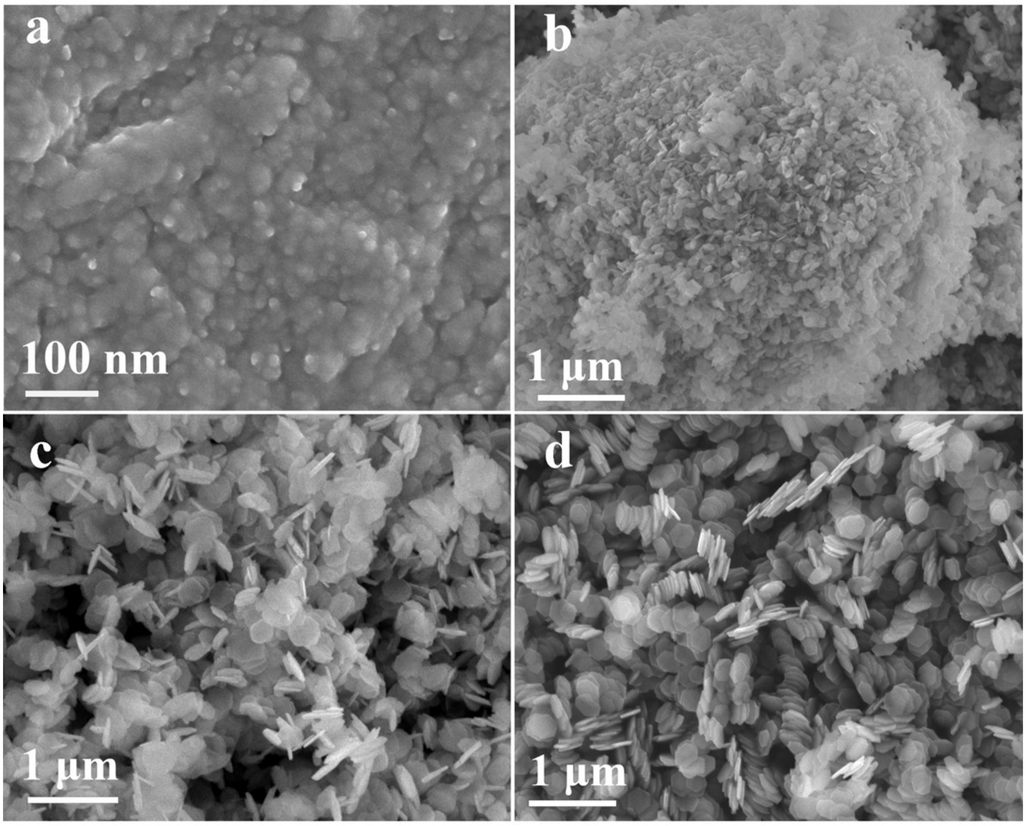

Fig. S5 SEM images of α-Fe_2O_3 HNP obtained with 56 mmol H_2O at reaction time: (a) 2 h, (b) 6 h, (c) 12 h, (d) 20 h.

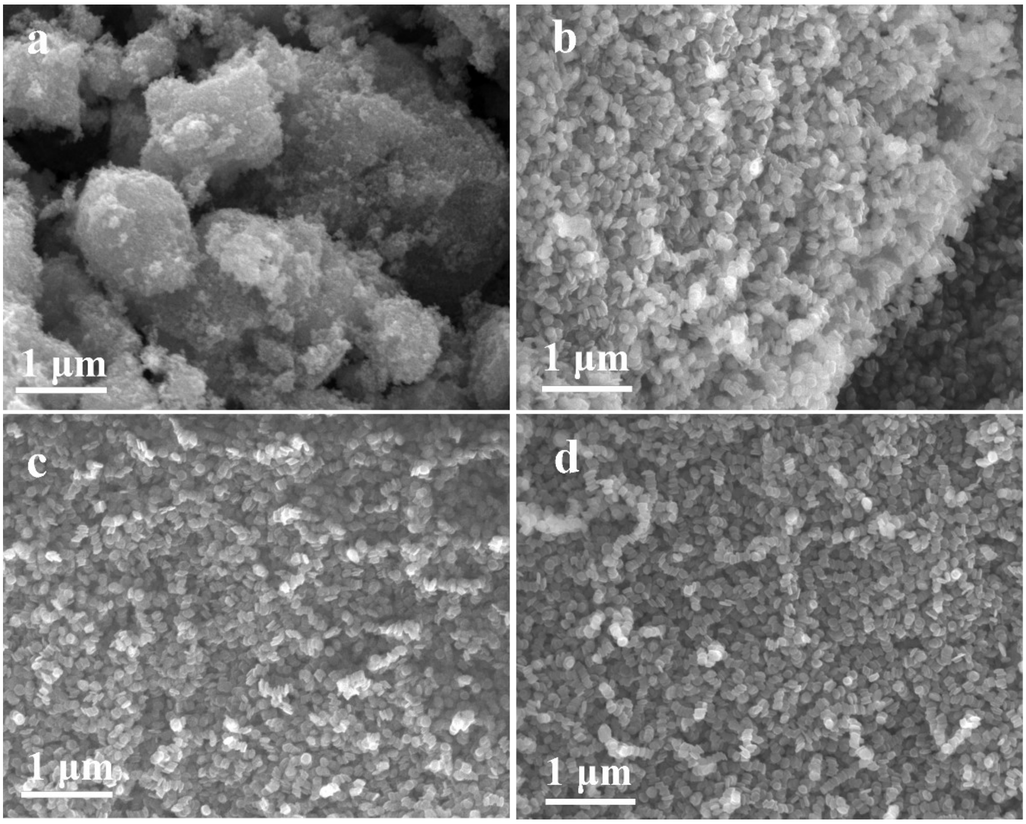

Fig. S6 SEM images of α-Fe_2O_3 SSHNP obtained with 222 mmol H_2O at reaction time (a) 3 h, (b) 6 h, (c) 12 h, (d) 21 h

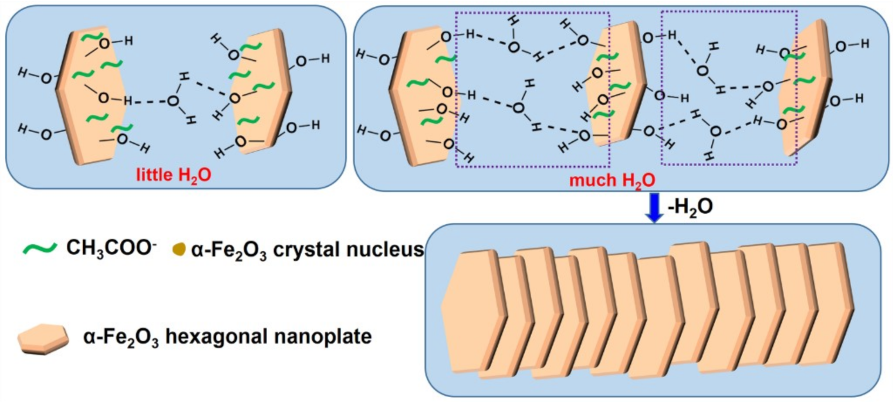

Fig. S7 Schematic diagram of hydrogen bond and dehydration process between α-Fe_2O_3 {001} facets.