## Heterogeneous Photo-Fenton Reaction on Hematite $(\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) {104}, {113} and {001} Surface Facets

J. Y. T. Chan,<sup>a, b</sup> S. Y. Ang,<sup>a, b</sup> E. Y. Ye, <sup>a</sup> M. Sullivan<sup>c</sup>, J. Zhang,<sup>c, \*</sup> and M. Lin<sup>a, \*</sup>

<sup>a</sup> Institute of Materials Research and Engineering, A\*STAR (Agency for Science, Technology and Research), 3 Research Link, S117602, Singapore

<sup>b</sup> School of Applied Science, Temasek Polytechnic, 21 Tampines Avenue 1, S529757, Singapore

<sup>c</sup> Institute of High Performance Computing, A\*STAR (Agency for Science, Technology and Research), 1 Fusionopolis Way #16-16 Connexis S138632, Singapore

\*Email: zhangj@ihpc.a-star.edu.sg, Tel.: 65-6419 1340; <u>m-lin@imre.a-star.edu.sg</u>, Tel.: 65-6874 5374, Fax: 65-6874 4778.



Fig. S1. Concentration of MB Vs Absorption of the solution.



Fig. S2. HRTEM image of an  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> hexagonal nanoplate particle.



Fig. S3. F 1s XPS spectra obtained from hexagonal bipyramid particles (a) after washing 1 time with water; (b) after washing 3 times; (c) after washing 5 times; (d) after washing 7 times; (e) after wash 10 times; and (f) after calcined at 400 °C.



Fig. S4. O 1s XPS spectra obtained from hexagonal bipyramid particles (a) after washing 1 time with water; (b); (c) after washing 3 times; (d) after washing 5 times; (e) after washing 10 times; and (f) after calcined at 400 °C.



Fig. S5. Cl 2p XPS spectra obtained from (a) rhombohedral; (b) hexagonal bipyramid and (c) hexagonal bipyramid particles after calcined at 400 °C.



Fig. S6. Indirect optical band gap measurement of rhombohedral particles.



Fig. S7. Indirect optical band gap measurement of hexagonal bipyramid particles.



Fig. S8. Indirect optical band gap measurement of hexagonal nanoplate particles.



Fig. S9. Enlargement of Fig. 5 in the main manuscript. The degradation efficiency of Methylene Blue was obtained under different reaction conditions over  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> nanocrystals with a rhombohedral shape.

Two experimental conditions were performed by increasing the volume of MB solution from 15 ml to 50 mL, while  $H_2O_2$  volume was reduced from 15 mL to 0.8 mL in the first experiment. In  $2^{nd}$  experiment, we have decreased the concentration of MB to 23 mg/L and volume of  $H_2O_2$  to 0.3 mL.



**Fig. S10.** Photo-catalytic degradation of Methylene Blue (blue) rhombohedron, (red) hexagonal bipyramid; (green) hexagonal nanoplate. Experimental conditions: MB concentration: 120 mg/L; 30% H2O2: 0.8 mL; reaction time 360 min.



**Fig. S11.** Photo-catalytic degradation of Methylene Blue (blue) rhombohedron, (red) hexagonal bipyramid; (green) hexagonal nanoplate. Experimental conditions: MB concentration: 23 mg/L; 30% H<sub>2</sub>O<sub>2</sub>: 0.3 mL; reaction time 180 min.

The normalized reaction constants were listed below. The order of reaction sequence is in agreement with the others with difference reaction conditions. This indicates that order of activities can be repeated when we keep the same experiment conditions.

MB	MB	30% H2O2	Catalyst	{113}	{104}	{001}
volume	concentration	(mL)				
15	50 mg/L	15	3 mg	3.7×10-4	3.2×10-4	1.7×10-4
50	120 mg/L	0.8	10 mg	3.3×10-4	1.9×10-4	1.6×10-4
50	23 mg/L	0.3	2 mg	1.2×10-2	7.2×10 <sup>-3</sup>	3.3×10 <sup>-4</sup>