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Supporting Information

High-Indexed Pt₃Fe Nanocatalysts and Their Enhanced Catalytic Performance in Dual Organic Reactions

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Table S1 ICP-OES measurement results.

Name & Replicates	Pt(mg/L)	Fe(mg/L)	W or Cr (mg/L)	Molar Ratio	Pt/Fe
Pt-Fe concave nanocubes by using W(CO) ₆					
Replicate 1	7.712	0.739	0.269 (W)	2.99	
Replicate 2	6.998	0.665	0.242 (W)	3.01	
Replicate 3	4.632	0.449	0.123 (W)	2.95	
Replicate 4	5.225	0.500	0.166 (W)	2.99	
Replicate 5	5.207	0.497	0.158 (W)	3.00	
Replicate 6	5.462	0.521	0.180 (W)	3.00	
Average				2.99	75.0/25.0
Pt-Fe nanocubes by using W(CO) ₆					
Replicate 1	6.302	0.624	0.192 (W)	2.89	
Replicate 2	6.775	0.653	0.217 (W)	2.97	
Replicate 3	5.847	0.579	0.177 (W)	2.89	
Replicate 4	6.223	0.601	0.197 (W)	2.96	
Replicate 5	5.343	0.520	0.167 (W)	2.94	
Replicate 6	5.862	0.563	0.189 (W)	2.98	
Average				2.94	74.6/25.4
Pt-Fe concave nanocubes by using Cr(CO) ₆					
Replicate 1	6.338	0.585	0.229 (Cr)	3.10	
Replicate 2	5.293	0.457	0.180 (Cr)	3.32	
Replicate 3	7.699	0.713	0.276 (Cr)	3.09	
Replicate 4	4.073	0.387	0.146 (Cr)	3.01	
Replicate 5	4.763	0.448	0.173 (Cr)	3.04	
Replicate 6	4.513	0.434	0.165 (Cr)	2.98	
Replicate 7	7.044	0.666	0.256 (Cr)	3.03	
Average				3.08	75.5/24.5

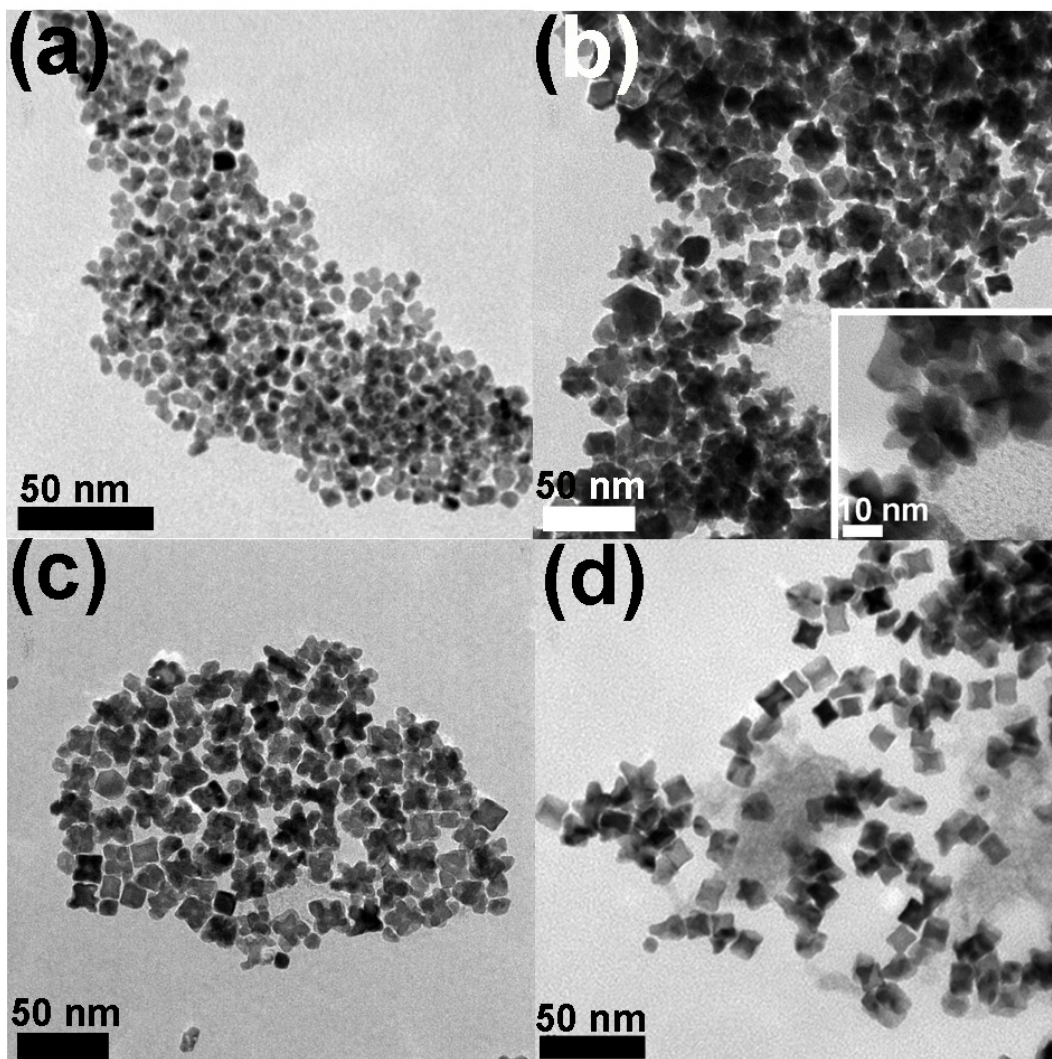


Figure S1. TEM images of Pt-Fe nanocrystals grown in early stage from a mixture of oleylamine and oleic acid (10:1 in volume) at 240 °C. Samples were collected in different reaction times: (a) 30 s; (b) 1 min; (c) 1.5 min; and (d) 2 min.

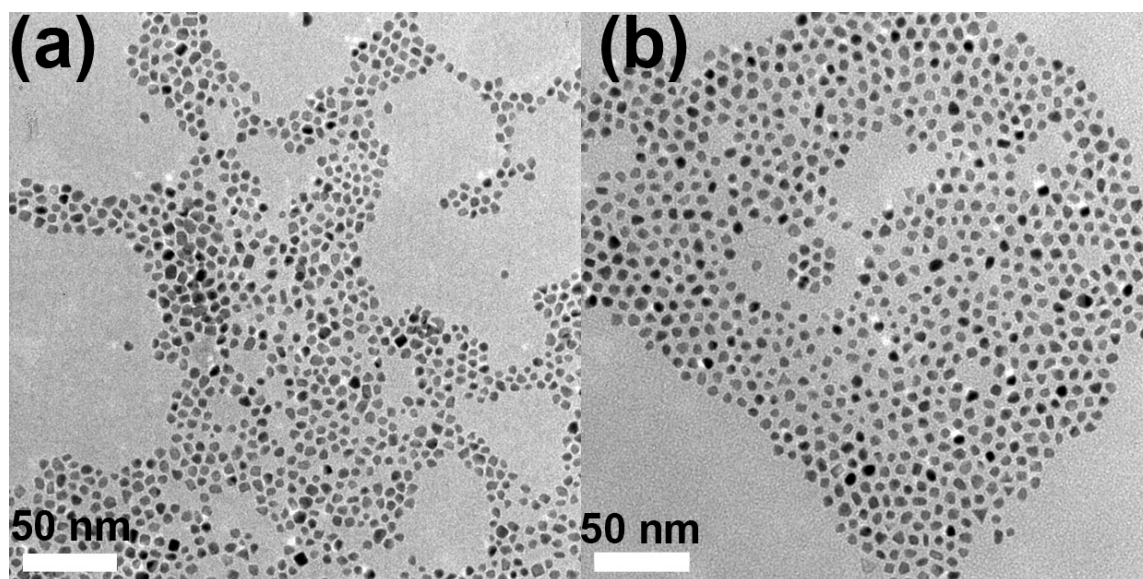
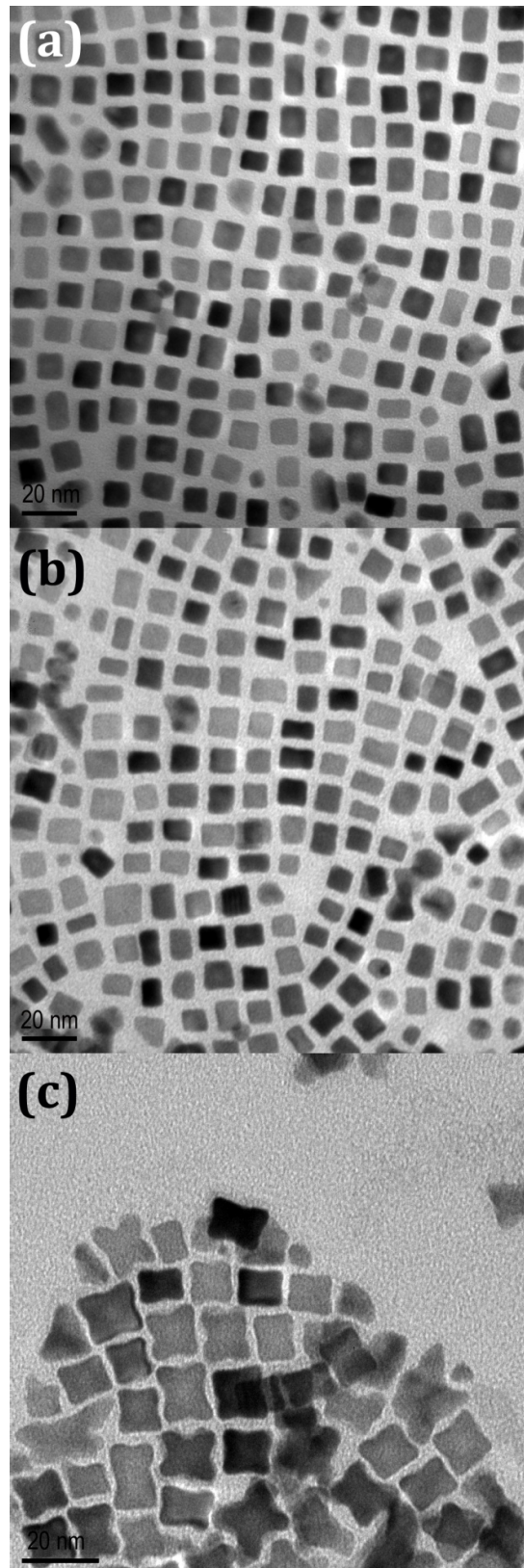


Figure S2. TEM images of Pt-Fe nanoparticles synthesized under similar conditions for the Pt_3Fe concave nanocubes but in the presence of amine and acid with different lengths of hydrocarbon-chains: (a) octylamine; (b) lauric acid.

Figure S3. (next page) TEM images of Pt-Fe nanocrystals grown for 40 min under the typical synthetic conditions (see Experimental Section), except for the following variation in each case: (a) the volume ratio of oleylamine/oleic acid was 4:1 and $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ was used as Fe-precursor; (b) the volume ratio of oleylamine/oleic acid was 4:1 and PtCl_4 was used as Pt-precursor; (c) the amount of $\text{Pt}(\text{acac})_2$ precursor was reduced (13 mg).



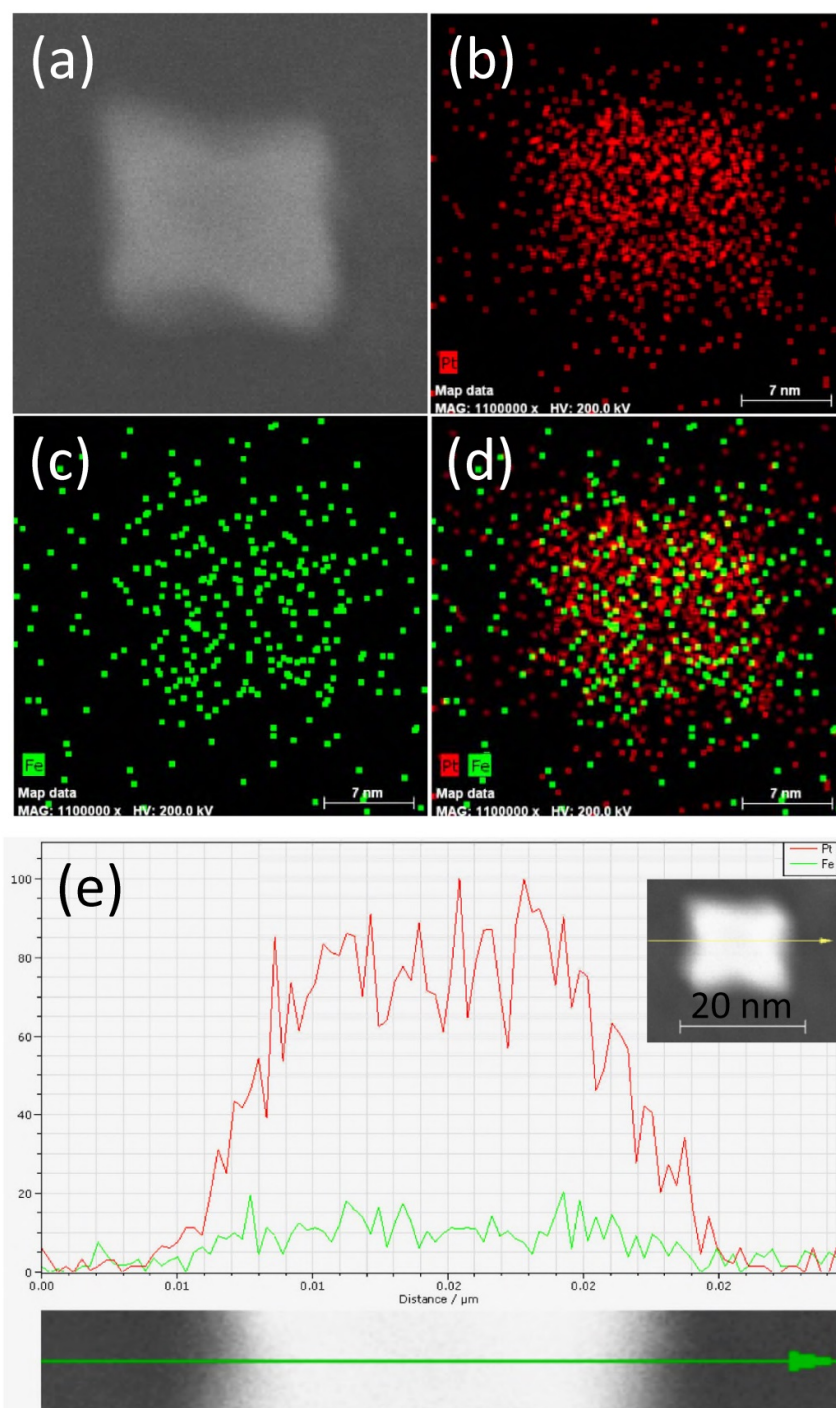


Figure S4. (a), STEM image of a selected concave nanocube; (b)-(d), STEM elemental maps of Pt (b, red), Fe (c, green) and Pt and Fe overlap (d) on the individual concave nanocube; (e), HAADF-STEM-EDS line scan profile of an individual concave nanocube (red line, Pt; green line, Fe; the inset is an STEM image of the selected concave nanocube).

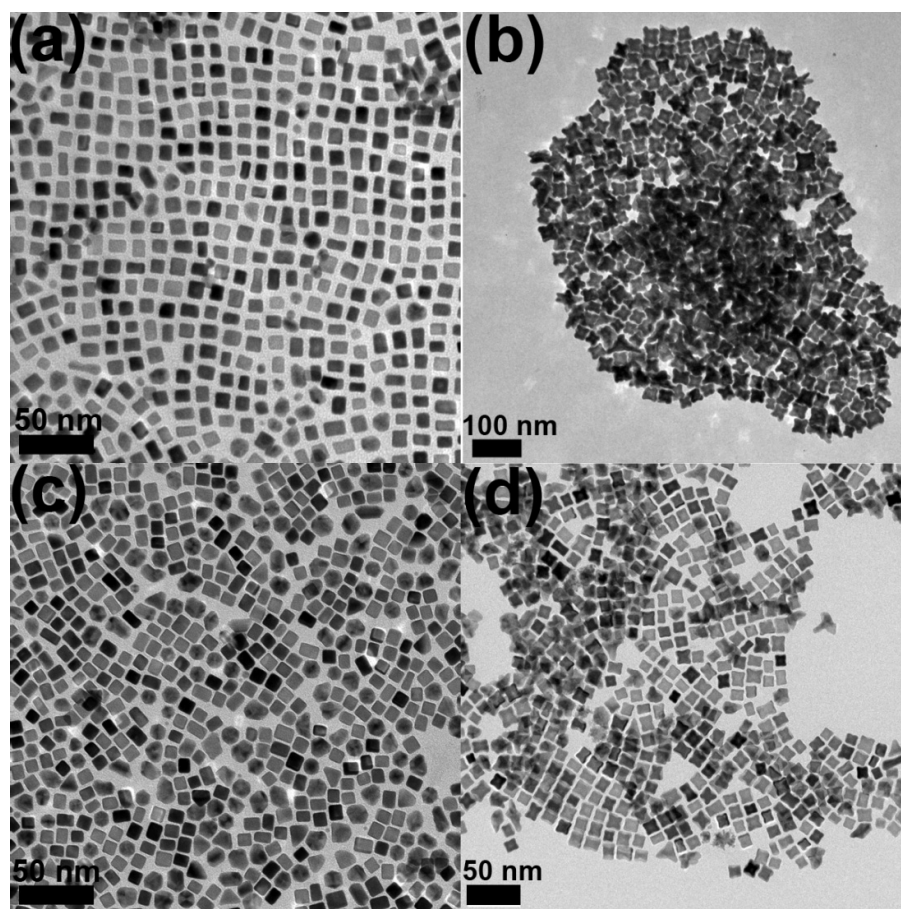


Figure S5. TEM images of NCs employed as the references to compare with Pt₃Fe concave nanocubes on the catalytic performances: (a) 10 nm Pt₃Fe nanocubes, (b) 20 nm Pt₃Fe concave nanocubes, (c) 10 nm Pt nanocubes; and (d) 10 nm Pt₃Fe concave nanocubes collected after the catalytic reusability test.

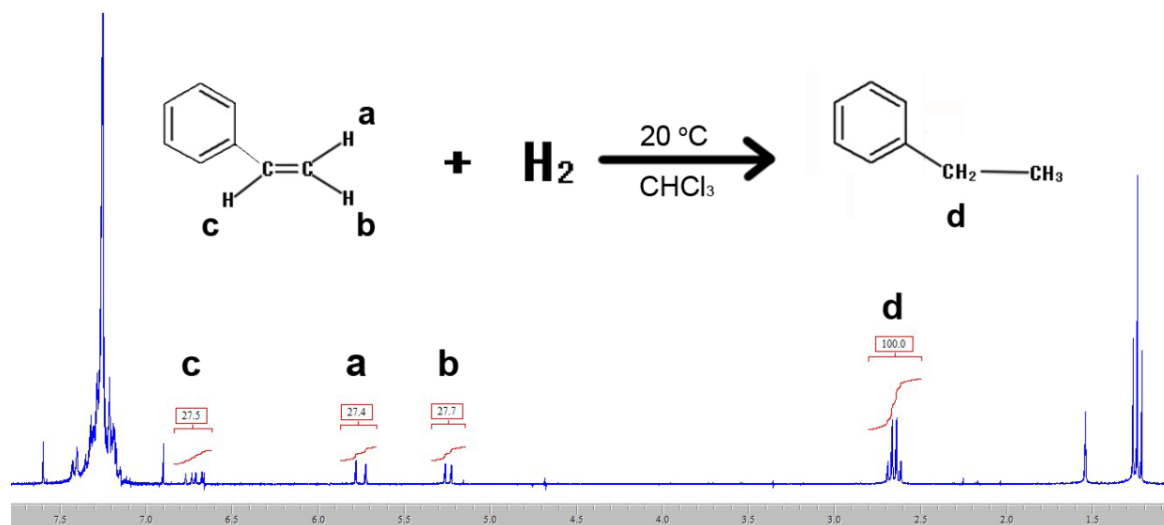


Figure S6. ^1H NMR (300 MHz, CDCl_3) of the reaction solution of styrene (reactant) and ethylbenzene (product) extracted during the catalytic reaction for the study of composition and conversion.

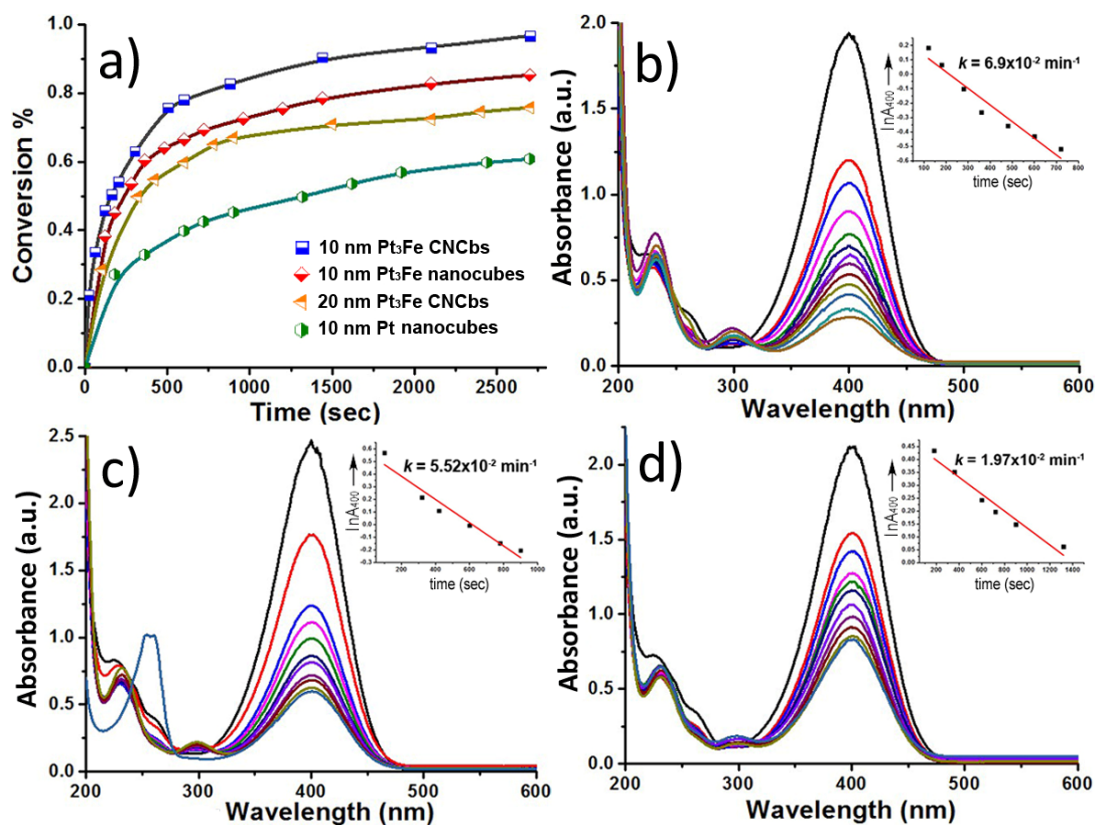


Figure S7. (a) the conversion of 4-nitrophenol versus time plot; continuous UV-Vis absorption spectra of the reduction of 4-nitrophenol in the presence of (b) 10 nm Pt₃Fe nanocubes, (c) 20 nm Pt₃Fe concave nanocubes, (d) 10 nm Pt nanocubes with the insets showing the plots of logarithm of the peak absorbance at 400 nm versus reduction time as well as the rate constants obtained from the slopes in the unit of min⁻¹.