

Ferrocene functionalized graphene: preparation, characterization and efficient catalyst for thermal decomposition of TKX-50

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Table S1 Contents of ferrocene functionalized graphene characterized using and ICP

Catalysts	Elemental analysis			ICP analysis
	C	H	N	Fe
G-550-Fe	39.22	4.76	5.25	1.03
G-551-Fe	38.71	4.55	4.39	2.64
G-602-Fe	46.35	4.44	5.23	4.46
G-792-Fe	40.02	4.50	4.93	1.96
G-902-Fe	44.16	4.71	3.82	3.38

Table S2 Decomposition peak temperature of TKX-50 catalyzed by ferrocene functionalized graphene

Catalysts	$T_p/^\circ\text{C}$	$T_p/^\circ\text{C}$			
		$\beta=5^\circ\text{C}\cdot\text{min}^{-1}$	$\beta=10^\circ\text{C}\cdot\text{min}^{-1}$	$\beta=15^\circ\text{C}\cdot\text{min}^{-1}$	$\beta=20^\circ\text{C}\cdot\text{min}^{-1}$
/	T_{LDP}	232.3	239.9	245.1	248.5
	T_{HDP}	260.8	268.0	272.9	275.1
G-792-Fe	T_{LDP}	194.9	203.6	208.3	211.7
	T_{HDP}	207.5	217.5	223.4	228.1
G-550-Fe	T_{LDP}	199.9	208.2	210.9	215.3
	T_{HDP}	220.5	233.6	238.3	242.5
G-602-Fe	T_{LDP}	195.8	203.9	208.2	212.1
	T_{HDP}	215.8	225.9	231.9	237.6
G-551-Fe	T_{LDP}	201.1	209.0	214.5	218.1
	T_{HDP}	227.0	238.7	245.7	250.0
G-902-Fe	T_{LDP}	200.4	208.2	214.2	216.2
	T_{HDP}	221.6	232.8	243.0	246.7

Table S3 Kinetic parameters of TKX-50 calculated by traditional Kissinger and Ozawa methods

Catalysts	$T_p/^\circ\text{C}$	Kissinger			Ozawa	
		$E_a/\text{kJ}\cdot\text{mol}^{-1}$	$\text{Lg}(A/\text{s}^{-1})$	r	$E_a/\text{kJ}\cdot\text{mol}^{-1}$	r
/	T_{LDP}	178.2	16.2	0.999	177.5	0.999
	T_{HDP}	221.4	19.5	0.998	219.1	0.998
G-792-Fe	T_{LDP}	147.5	14.3	0.999	147.8	0.999
	T_{HDP}	127.3	11.6	0.999	128.8	0.999
G-550-Fe	T_{LDP}	168.8	16.5	0.993	168.1	0.993
	T_{HDP}	123.8	10.8	0.992	125.7	0.993

G-602-Fe	T_{LDP}	154.6	15.1	0.999	154.5	0.999
	T_{HDP}	125.3	11.1	0.998	127.1	0.998
G-551-Fe	T_{LDP}	149.2	14.2	0.999	149.5	0.999
	T_{HDP}	121.5	10.4	0.999	123.6	0.999
G-902-Fe	T_{LDP}	154.4	14.9	0.995	154.5	0.996
	T_{HDP}	105.1	8.7	0.994	107.9	0.995

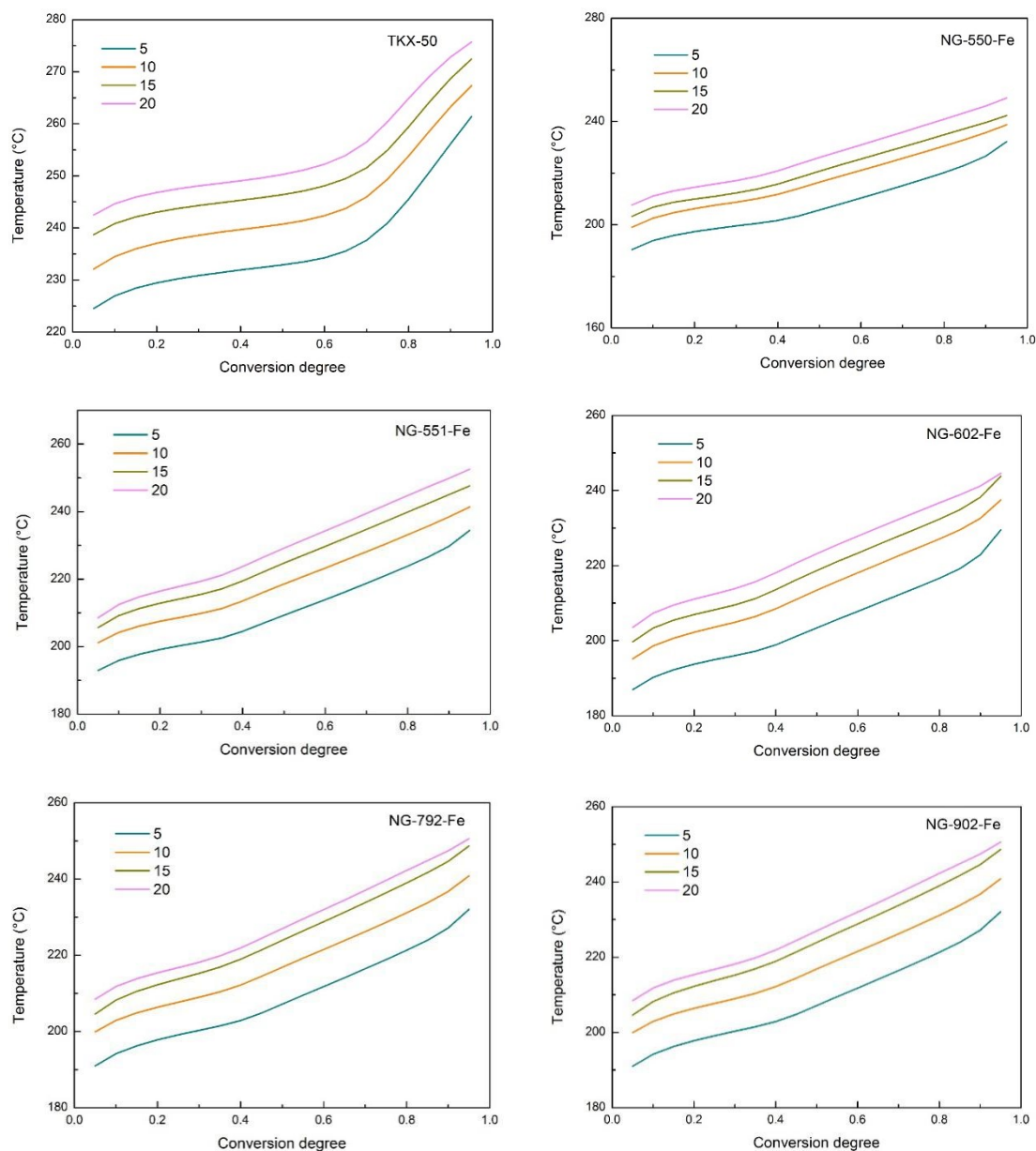


Fig. S1 Conversion degree-temperature curves of TKX-50 catalyzed with ferrocene functionalized graphene at different heating rates

Table S4 Kinetic parameters of TKX-50 mixed with graphene functionalized ferrocene obtained using nonlinear Kissinger model

α	TKX-50			TKX-50+G-550-Fe			TKX-50+G-551-Fe			TKX-50+G-602-Fe			TKX-50+G-792-Fe			TKX-50+G-902-Fe		
	E_a	LgA	r	E_a	LgA	r	E_a	LgA	r	E_a	LgA	r	E_a	LgA	r	E_a	LgA	r
0.05	153.2	13.8	0.996	143.1	14.0	0.999	156.8	15.4	0.999	145.8	14.4	1.000	157.3	15.7	1.000	140.4	13.6	1.000
0.10	158.0	14.3	0.997	144.7	14.0	0.999	150.2	14.6	1.000	143.4	14.0	1.000	150.5	14.8	1.000	139.8	13.4	1.000

0.15	161.2	14.6	0.998	146.8	14.2	0.998	147.3	14.2	1.000	143.2	13.9	1.000	147.8	14.4	1.000	140.3	13.4	1.000
0.20	164.3	14.8	0.998	148.6	14.3	0.997	145.5	13.9	1.000	143.5	13.9	1.000	145.9	14.2	1.000	140.6	13.4	0.999
0.25	165.0	14.9	0.999	149.0	14.3	0.996	143.7	13.7	1.000	143.2	13.8	1.000	144.3	13.9	1.000	140.4	13.3	0.999
0.30	166.6	15.0	0.999	147.3	14.1	0.996	141.4	13.4	1.000	141.4	13.5	0.999	142.1	13.7	1.000	138.8	13.1	0.998
0.35	167.2	15.1	0.999	142.7	13.5	0.996	136.7	12.8	1.000	137.0	13.0	0.999	139.3	13.3	0.999	135.6	12.7	0.998
0.40	167.5	15.1	0.999	135.4	12.7	0.996	134.4	12.5	1.000	132.6	12.4	1.000	135.6	12.8	0.999	131.0	12.1	0.998
0.45	167.9	15.1	0.999	130.2	12.0	0.996	133.0	12.2	1.000	131.1	12.2	1.000	132.6	12.4	0.998	128.3	11.8	0.998
0.50	166.2	14.9	0.999	129.5	11.9	0.997	132.2	12.1	0.999	130.7	12.1	1.000	131.1	12.2	0.998	127.9	11.7	0.998
0.55	164.9	14.8	0.999	129.8	11.8	0.997	131.5	11.9	0.999	130.8	12.0	1.000	130.4	12.1	0.998	127.9	11.6	0.998
0.60	162.7	14.5	0.999	130.6	11.9	0.997	131.3	11.8	0.999	131.4	12.0	0.999	130.2	12.0	0.998	127.9	11.5	0.998
0.65	159.5	14.1	0.999	131.5	11.9	0.997	131.3	11.8	0.999	132.1	12.0	0.999	130.2	11.9	0.998	127.9	11.5	0.998
0.70	157.6	13.9	0.998	132.7	11.9	0.996	131.3	11.7	0.999	133.0	12.1	0.999	130.5	11.9	0.998	127.9	11.4	0.998
0.75	155.4	13.5	0.996	134.1	12.0	0.996	132.6	11.8	0.999	134.0	12.1	0.999	130.7	11.9	0.997	127.6	11.3	0.997
0.80	159.6	13.8	0.996	136.3	12.2	0.996	132.6	11.7	0.999	135.5	12.2	0.999	130.5	11.8	0.997	127.7	11.2	0.997
0.85	170.2	14.7	0.997	140.4	12.5	0.995	135.6	11.9	0.998	139.1	12.5	0.999	130.0	11.6	0.994	129.1	11.3	0.997
0.90	190.1	16.6	0.997	149.8	13.4	0.992	141.6	12.5	0.998	149.2	13.5	0.998	133.9	11.9	0.977	134.3	11.8	0.996
0.95	224.8	19.8	0.996	174.1	15.9	0.976	159.3	14.2	0.991	175.6	16.1	0.987	159.6	14.2	0.955	146.8	12.9	0.992

Table S5 Kinetic parameters of TKX-50 catalyzed by ferrocene functionalized graphene obtained using nonlinear Flynn-Wall-Ozawa model

a	TKX-50		TKX-50+G-550-Fe		TKX-50+G-551-Fe		TKX-50+G-602-Fe		TKX-50+G-792-Fe		TKX-50+G-902-Fe	
	E_a	r	E_a	r	E_a	r	E_a	r	E_a	r	E_a	r
0.05	153.7	0.997	143.6	0.999	156.6	0.999	146.0	1.000	157.0	1.000	141.1	1.000
0.10	158.3	0.998	145.1	0.999	150.3	1.000	143.8	1.000	150.6	1.000	140.5	1.000
0.15	161.4	0.998	147.1	0.998	147.6	1.000	143.6	1.000	148.1	1.000	141.0	1.000
0.20	164.3	0.998	148.9	0.997	146.0	1.000	144.0	1.000	146.2	1.000	141.3	0.999
0.25	165.0	0.999	149.2	0.996	144.3	1.000	143.7	1.000	144.7	1.000	141.1	0.999
0.30	166.5	0.999	147.6	0.996	142.1	1.000	142.0	0.999	142.7	1.000	139.6	0.999
0.35	167.1	0.999	143.3	0.996	137.7	1.000	137.9	0.999	140.0	0.999	136.6	0.998
0.40	167.4	0.999	136.4	0.997	135.5	1.000	133.7	1.000	136.5	0.999	132.3	0.998
0.45	167.7	0.999	131.5	0.997	134.2	1.000	132.4	1.000	133.7	0.999	129.7	0.998
0.50	166.2	0.999	130.8	0.997	133.5	1.000	132.0	1.000	132.3	0.998	129.3	0.998
0.55	165.0	0.999	131.2	0.997	132.8	0.999	132.2	1.000	131.7	0.998	129.4	0.998
0.60	162.9	0.999	132.0	0.997	132.7	1.000	132.7	1.000	131.5	0.998	129.4	0.998
0.65	159.9	0.999	132.9	0.997	132.8	0.999	133.4	0.999	131.6	0.998	129.5	0.998
0.70	158.1	0.998	134.1	0.997	132.8	0.999	134.3	0.999	131.9	0.998	129.5	0.998
0.75	156.1	0.997	135.5	0.997	134.1	0.999	135.3	0.999	132.0	0.998	129.3	0.998
0.80	160.1	0.997	137.5	0.996	134.1	0.999	136.7	0.999	132.0	0.997	129.4	0.997
0.85	170.3	0.997	141.5	0.995	137.0	0.999	140.2	0.999	131.5	0.995	130.8	0.997
0.90	189.3	0.997	150.5	0.993	142.7	0.998	149.9	0.998	135.3	0.980	135.8	0.996
0.95	222.4	0.996	173.7	0.978	159.6	0.992	175.0	0.988	159.9	0.959	147.7	0.993