

Supplementary Information

Use of Biodiesel Press Cake Waste to Prepare Fe/Carbon Reactive Composites for Environmental Applications: Removal of Hazardous Cr^{VI} Contaminants

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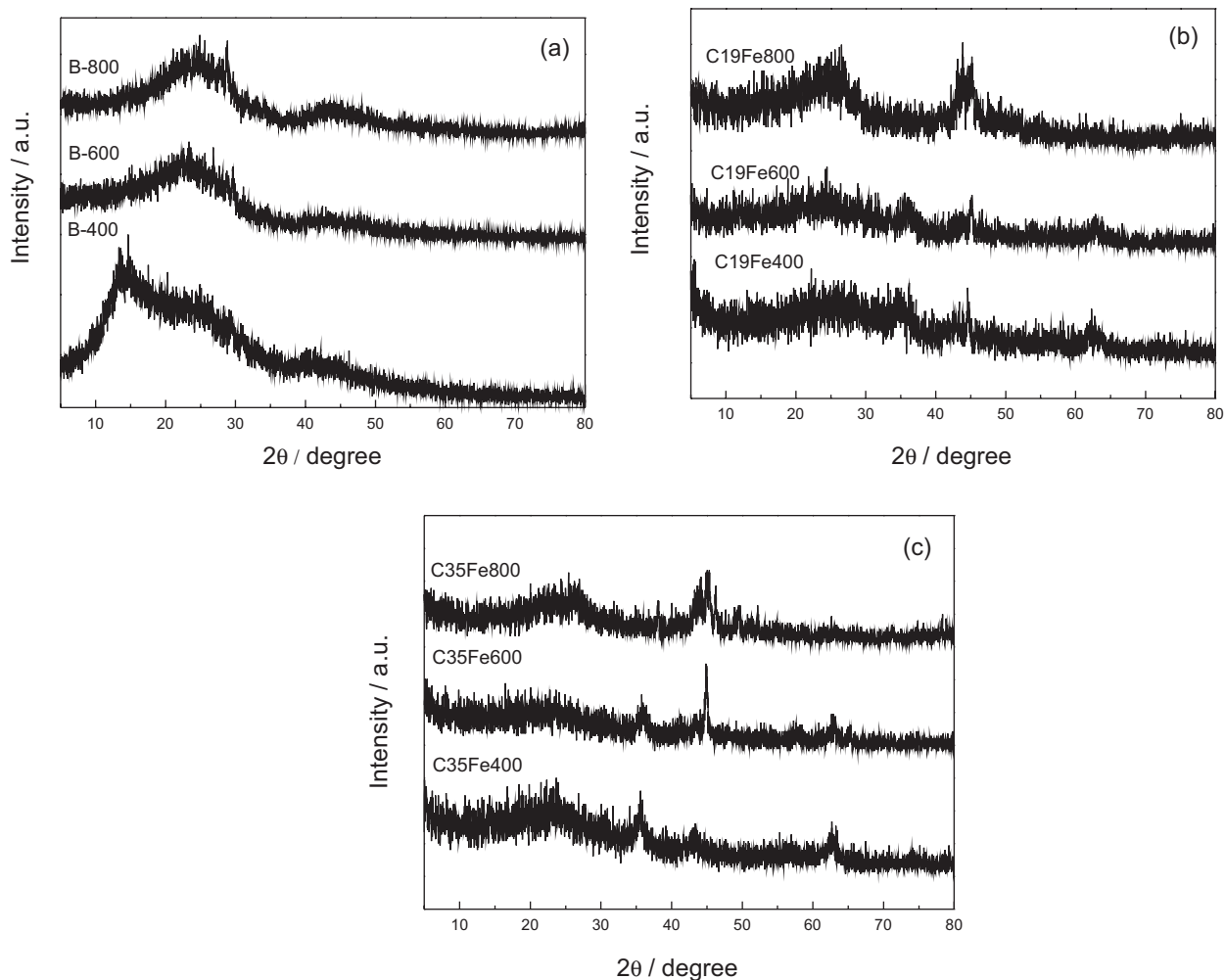


Figure S1. X-ray diffractograms of composites with (a) 0; (b) 19; (c) 35 wt.% Fe pyrolyzed at 400, 600 and 800 °C.

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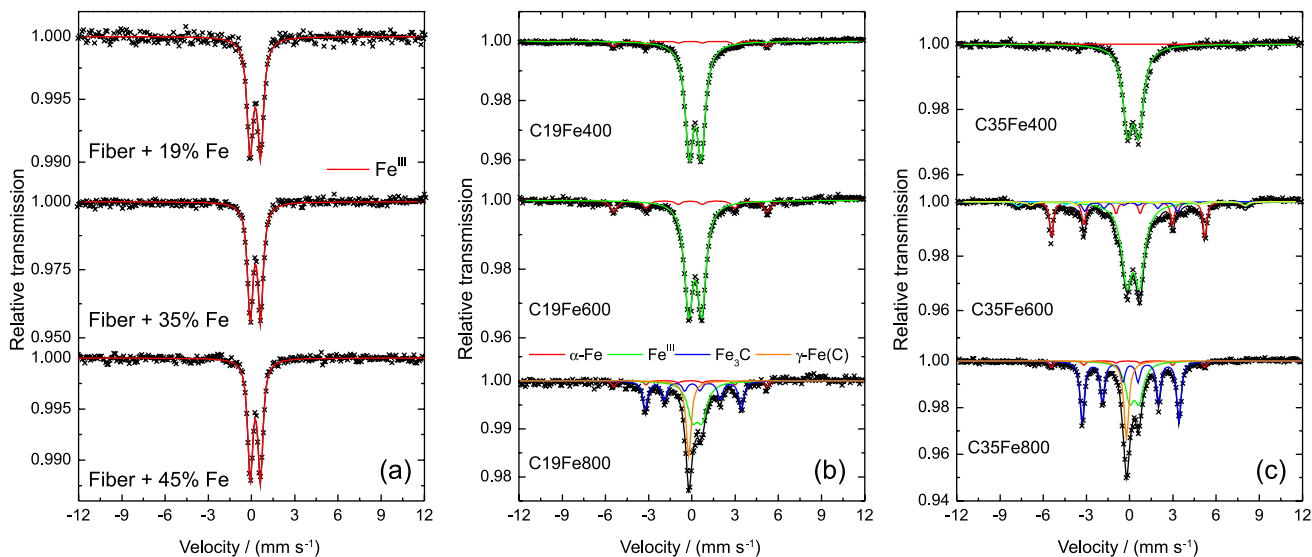


Figure S2. Mössbauer spectra. (a) Press cake impregnated with 19, 35 and 45% Fe; composites pyrolyzed at 400, 600 and 800 °C with (b) 19 and (c) 35% Fe.

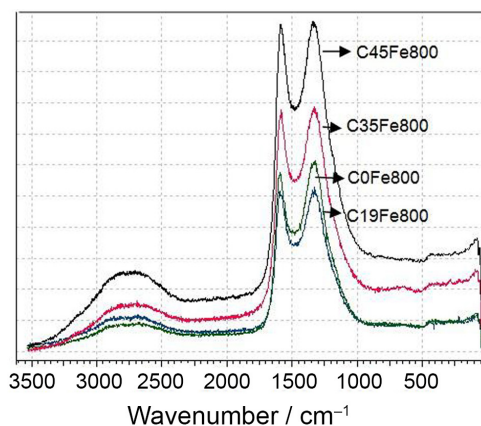


Figure S3. Raman spectra of samples with 0, 19, 35 and 45% Fe pyrolyzed at 800 °C.

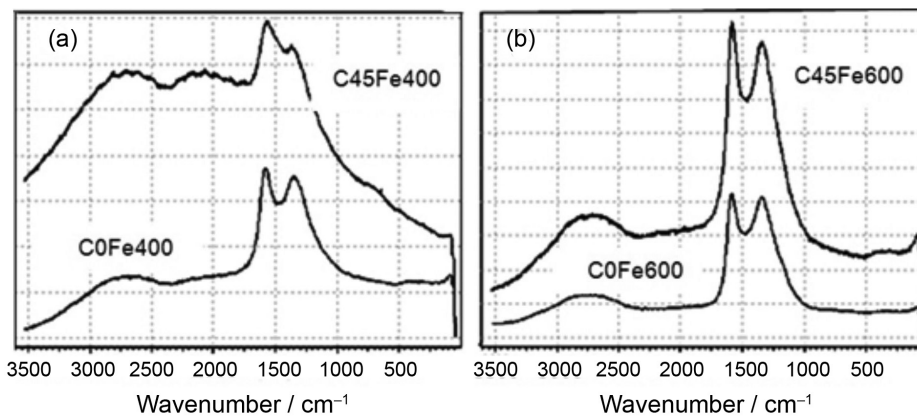


Figure S4. Raman spectra of samples with 0 and 45% Fe pyrolyzed at (a) 400 °C; (b) 600 °C.

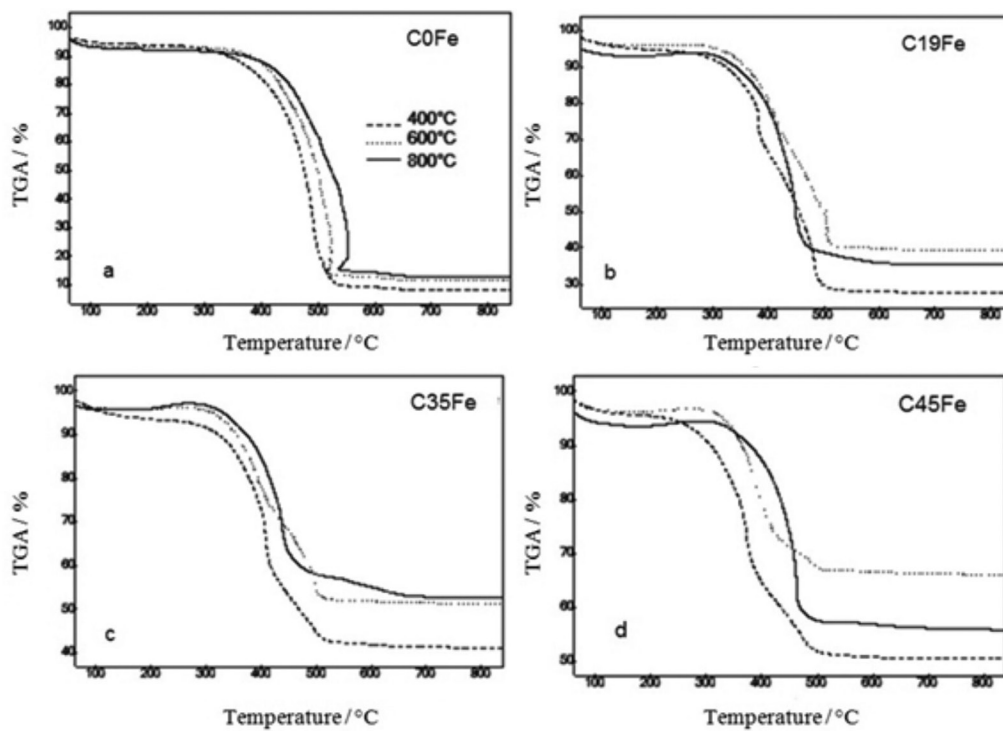


Figure S5. Thermogravimetric analyses in air of samples with (a) 0; (b) 19%; (c) 35%; (d) 45% Fe previously pyrolyzed at different temperatures.

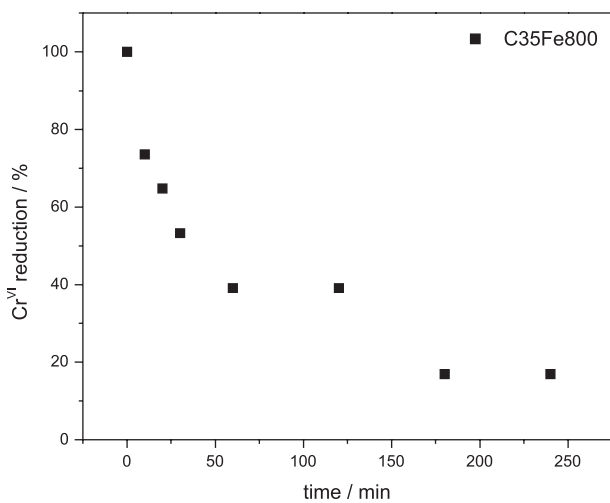


Figure S6. Cr^{VI} removal in the presence of the composite C35Fe800 by the diphenylcarbazide method.

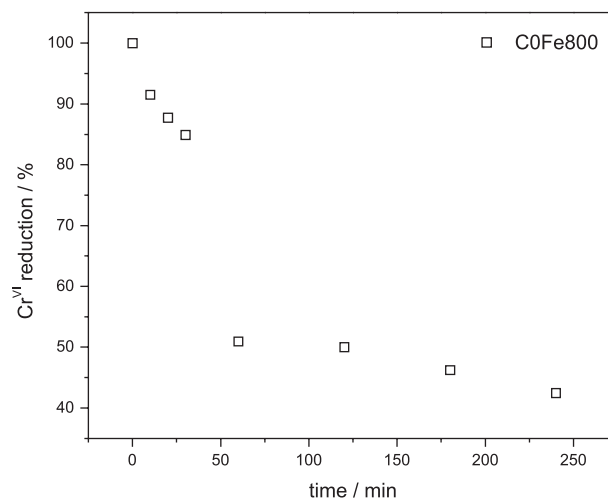


Figure S7. Cr^{VI} removal in the presence of the composite C0Fe800 by the diphenylcarbazide method.

Table S1. Mössbauer hyperfine parameters for the composites containing 19, 35 and 45% Fe and pyrolyzed at 400, 600 and 800 °C

Sample	Phase	$\delta^a \pm 0.05 / (\text{mm s}^{-1})$	$\Delta Q^{b,c} \pm 0.05 / (\text{mm s}^{-1})$	$B_{\text{HF}}^d \pm 0.7 / \text{T}$	$RA^e \pm 1 / \%$
C19Fe400	α -Fe	0.00	0.00	33.0	7
	Fe ^{III}	0.33	0.83	–	93
C19Fe600	α -Fe	0.00	0.00	33.0	15
	Fe ^{III}	0.33	0.90	–	85
C19Fe800	α -Fe	0.00	0.00	33.0	5
	Fe ^{III}	0.47	0.66	–	39
	Fe ₃ C	0.16	0.06	20.6	33
	γ Fe(C)	-0.12	–	–	23
C35Fe400	Fe ^{III}	0.35	0.78	–	100
C35Fe600	α -Fe	0.00	0.00	33.0	21
	Fe ^{III}	0.35	0.89	–	63
	Fe ₃ C	0.16	0.20	20.0	8
	Fe ₃ O ₄	0.27	0.02	48.1	4
	Fe ₃ O ₄	0.66	0.01	46.0	4
C35Fe800	α -Fe	0.00	0.00	33.0	5
	Fe ^{III}	0.43	0.66	–	29
	Fe ₃ C	0.16	0.04	20.8	48
	γ Fe(C)	-0.12	–	–	18
C45Fe400	Fe ^{III}	0.35	0.89	–	83
	Fe ₃ O ₄	0.27	0.02	48.0	7
	Fe ₃ O ₄	0.66	0.01	45.0	10
C45Fe600	α -Fe	0.00	0.00	33.0	3
	Fe ^{III}	0.35	0.89	–	65
	Fe ₃ C	0.16	0.20	22.1	19
	Fe ₃ O ₄	0.26	0.01	48.5	6
	γ Fe(C)	0.66	0.01	45.4	7
C45Fe800	α -Fe	0.00	0.00	33.0	20
	Fe ^{III}	0.43	0.66	–	29
	Fe ₃ C	0.17	0.04	20.9	40
	γ Fe(C)	-0.09	–	–	11

^a δ : isomer shift with respect to α -Fe; ^bQ: quadrupole shift; ^c Δ : quadrupole splitting; ^d B_{HF} : hyperfine field; ^eRA: relative sub-spectral area.

Table S2. Magnetization measurements of samples containing 0, 19, 35 and 45 wt.% Fe and pyrolyzed at 400, 600 and 800 °C

Sample	Magnetization measurement / (emu g ⁻¹)		
	Carbonization temperature / °C		
	400	600	800
C0Fe	0.09	0.10	0.05
C19Fe	0.96	2.02	5.50
C35Fe	2.85	8.63	14.3
C45Fe	5.48	15.3	20.1

Table S3. Element content for composites pyrolyzed at 400, 600 and 800 °C

	Pyrolysis temperature / °C											
	400				600				800			
	Element content / (wt.%)											
	C	H	N	Others	C	H	N	Others	C	H	N	Others
C19Fe	46	3.6	5.4	45	59	1.0	3.0	37	58	1.2	1.8	39
C35Fe	41	3.6	5.4	50	37	1.8	3.2	58	50	1.5	1.5	47
C45Fe	44	3.1	5.9	47	33	1.5	3.5	62	45	1.2	1.8	52

Table S4. Characteristics of surface groups in the magnetic composites

Composite	Number of site / (mmol g ⁻¹)			
	pKa 5-7	pKa 8-11	Total	pH _{zpc}
C19Fe400	0.29	2.34	2.63	8
C45Fe400	–	3.35	3.35	8.2
C19Fe600	1.08	1.65	2.73	10.6
C35Fe600	0.28	1.76	2.04	8.8
C45Fe600	–	0.54	0.54	8.4
C19Fe800	0.21	1.99	2.20	9
C35Fe800	0.91	1.02	1.93	10.4
C45Fe800	3.08	3.12	6.20	10