

Electronic supplementary information (ESI)

**Reactive porous composites for chromium(VI) reduction applications based on Fe/carbon obtained from post-consumer PET and iron oxide.**

Lílian A. Carvalho, José D. Ardisson, Rochel M. Lago, Maria D. Vargas and

Maria Helena Araujo

Contents

**Fig. S1** (a) XDR pattern; (b) Mössbauer spectrum and (c) Raman spectrum of the hematite prepared by thermal treatment of iron(III) nitrate at 450 °C.

**Fig. S2** Profile of temperature along with the evolution of gases of  $\text{Fe}_{500}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{600}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  and  $\text{Fe}_{1000}/\text{C}_{\text{PET}}$  under argon atmosphere.

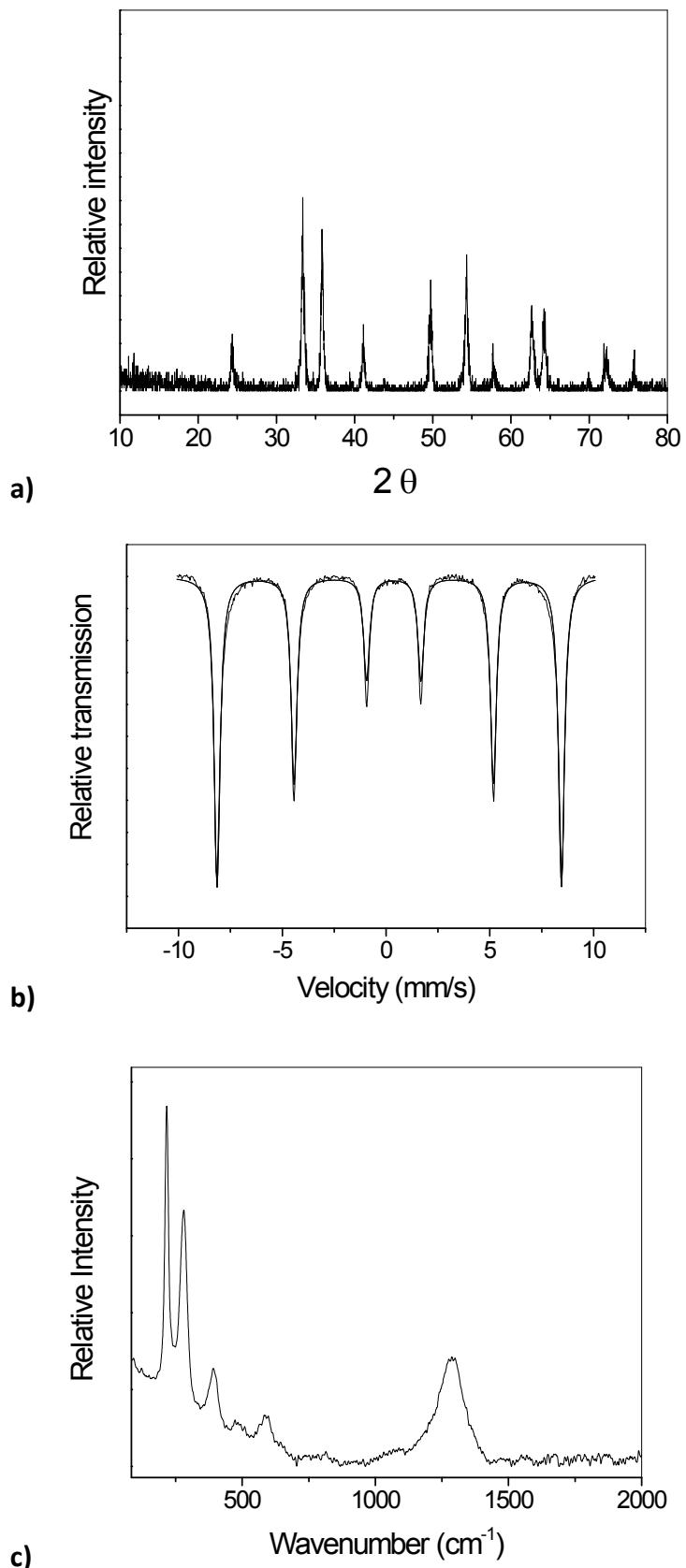
**Fig. S3** EDS mapping of (a)  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  and (b)  $\text{Fe}_{900}/\text{C}_{\text{PET}}$ .

**Fig. S4** Nitrogen adsorption and desorption isotherms obtained for (a)  $\text{Fe}_{500}/\text{C}_{\text{PET}}$ ; (b)  $\text{Fe}_{600}/\text{C}_{\text{PET}}$ ; (c)  $\text{Fe}_{800}/\text{C}_{\text{PET}}$ ; (d)  $\text{Fe}_{1000}/\text{C}_{\text{PET}}$  and surface area values.

**Fig. S5** Pore distribution in the  $\text{Fe}_{500}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{600}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  and  $\text{Fe}_{1000}/\text{C}_{\text{PET}}$  composites.

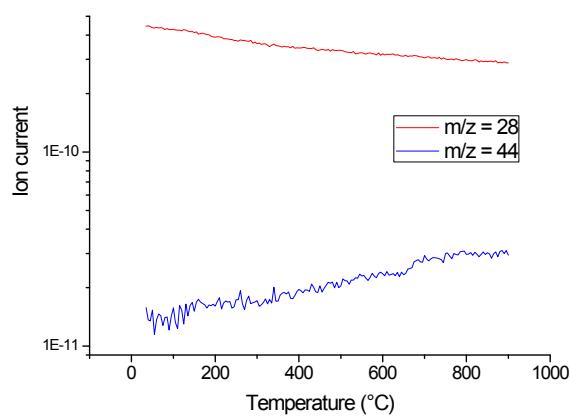
**Fig. S6** Magnetic separation of the  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  composite from a suspension in water.

**Table S1** Mössbauer hyperfine parameters of the composites.

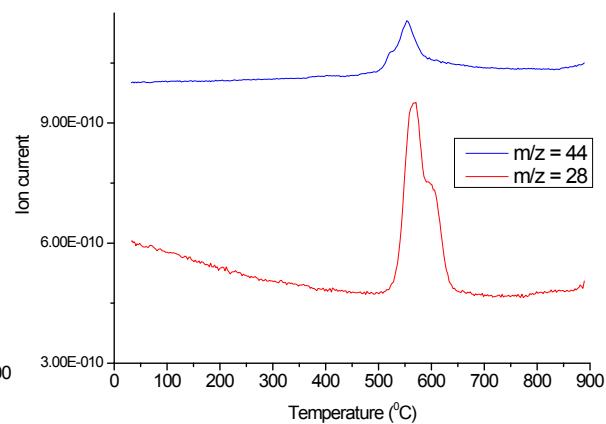


**Fig. S1** (a) XDR pattern; (b) Mössbauer spectrum and (c) Raman spectrum of the hematite prepared by thermal treatment of iron(III) nitrate at 450 °C. All the signals and bands are only related to hematite.

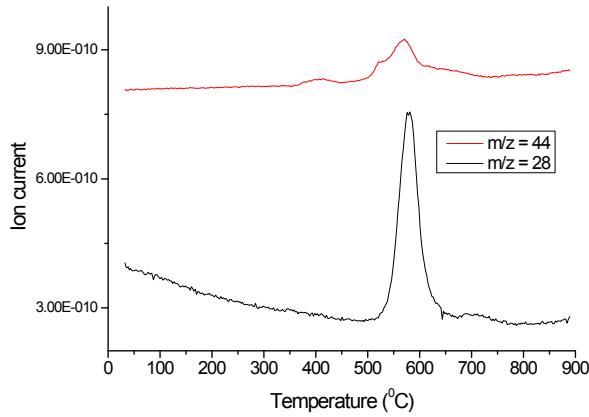
$\text{Fe}_{700}/\text{C}_{\text{PET}}$



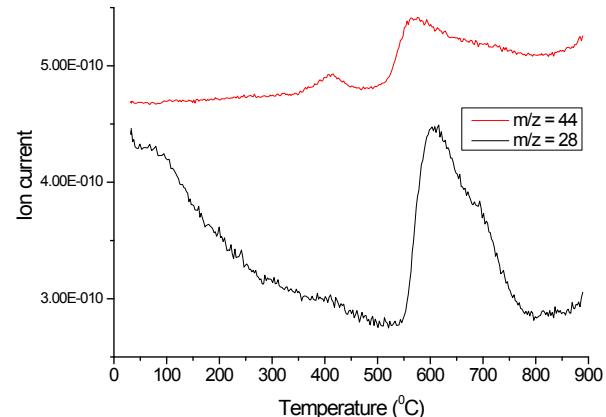
$\text{Fe}_{800}/\text{C}_{\text{PET}}$



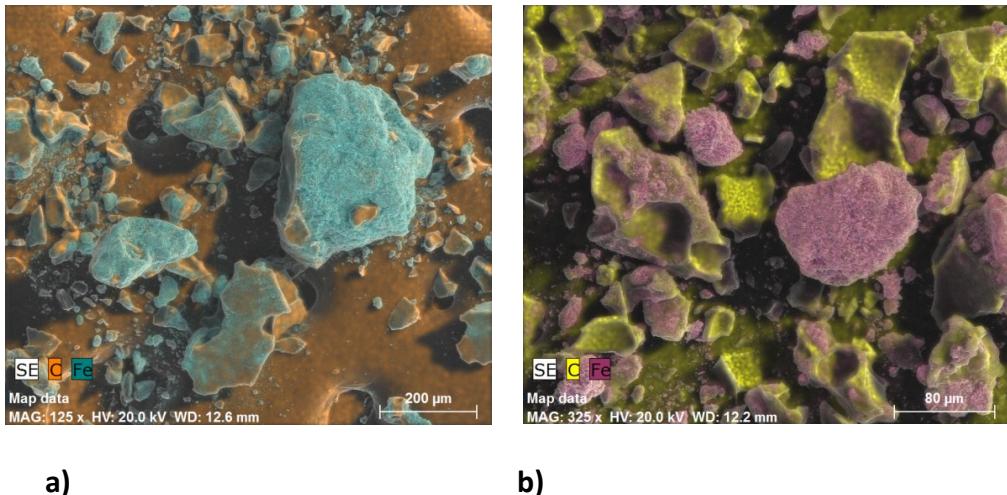
$\text{Fe}_{900}/\text{C}_{\text{PET}}$



$\text{Fe}_{1000}/\text{C}_{\text{PET}}$

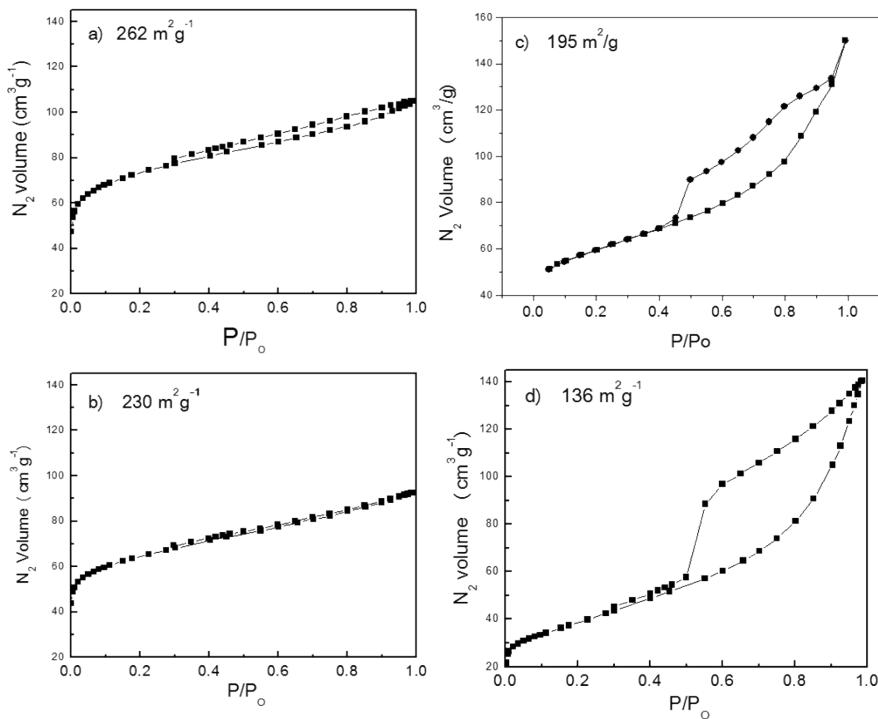


**Fig. S2** Profile of temperature along with the evolution of gases of  $\text{Fe}_{500}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{600}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  and  $\text{Fe}_{1000}/\text{C}_{\text{PET}}$  under argon atmosphere.

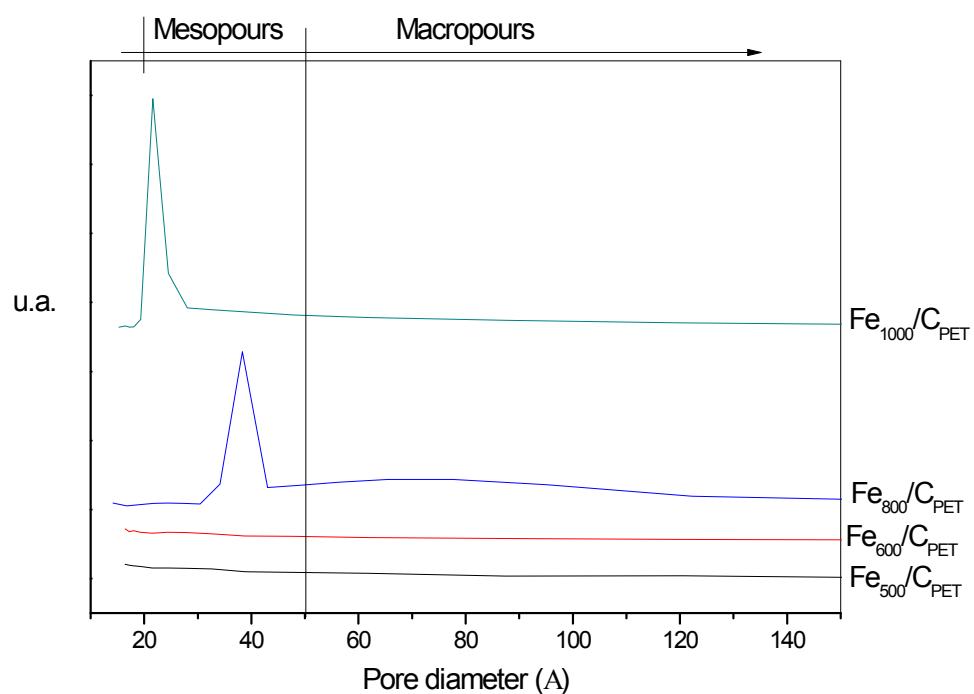


**Fig. S3** EDS mapping of (a)  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  and (b)  $\text{Fe}_{900}/\text{C}_{\text{PET}}$ .

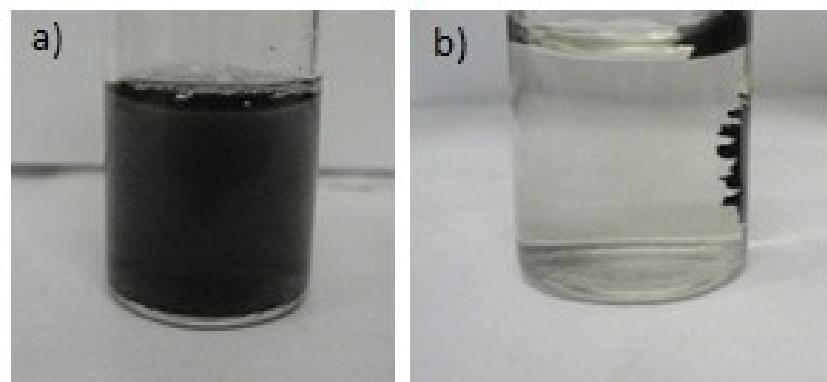
EDS mapping suggests that the Fe is homogeneously distributed throughout the particles, as it may be seen by the blue and pink colors in Fig. S2 (a) and (b), respectively, which shows the mapping of the elemental Fe in the material. The distribution of the carbon in the material is indicated by the orange and yellow colors in Fig. S2 (a) and (b).



**Fig. S4** Nitrogen adsorption and desorption isotherms obtained for (a)  $\text{Fe}_{500}/\text{C}_{\text{PET}}$ ; (b)  $\text{Fe}_{600}/\text{C}_{\text{PET}}$ ; (c)  $\text{Fe}_{800}/\text{C}_{\text{PET}}$ ; (d)  $\text{Fe}_{1000}/\text{C}_{\text{PET}}$  and the surface area values.



**Fig. S5** Pore distribution in the  $\text{Fe}_{500}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{600}/\text{C}_{\text{PET}}$ ,  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  and  $\text{Fe}_{1000}/\text{C}_{\text{PET}}$  composites.



**Fig. S6.** Magnetic separation of the  $\text{Fe}_{800}/\text{C}_{\text{PET}}$  composite from a suspension in water.

**Table S1** Mössbauer hyperfine parameters of the composites.

Material	Phase	$\delta \pm 0.05$ (mm/s)	$2\varepsilon/\Delta Q \pm 0.05$ (mm/s)	$B_{HF} \pm 0.5$ (Tesla)	Area $\pm 1$ (%)
$Fe_{500}/C_{PET}$	<b>mix <math>Fe_3O_4</math>,</b>	0.65	0.04	46.0	28
	$\gamma\text{-}Fe_3O_4$	0.25	-0.06	49.0	29
	$Fe^{3+}$	0.21	1.34	-	18
	$Fe^{2+}$	0.97	1.08	-	09
	<b>FeOOH</b>	0.63	0.13	38.4	16
<hr/>					
$Fe_{600}/C_{PET}$	<b>mix <math>Fe_3O_4</math>,</b>	0.53	0.04	45.6	27
	$\gamma\text{-}Fe_3O_4$	0.27	-0.06	49.2	26
	$Fe^{3+}$	0.34	1.62	-	15
	$Fe^{2+}$	0.97	1.40	-	15
	<b>FeOOH</b>	0.31	0.13	40.9	17
<hr/>					
$Fe_{700}/C_{PET}$	$\alpha\text{-}Fe$	0.0	0.0	33.0	23
	$Fe_3C$	0.17	0.02	20.8	69
	$\gamma\text{-}Fe(C)$	0.41	0.80	-	4
	$\gamma\text{-}Fe$	-0.20	-	-	4
<hr/>					
$Fe_{800}/C_{PET}$	$\alpha\text{-}Fe$	0,00	0,00	33,10	65
	$Fe_3C$	0,20	0,03	20,70	22
	$\gamma\text{-}Fe$	-0,09	-----	-----	13
<hr/>					
$Fe_{900}/C_{PET}$	$\alpha\text{-}Fe$	0.0	0.0	33.0	31
	$Fe_3C$	0.17	0.02	20.8	53
	$\gamma\text{-}Fe(C)$	0.39	0.58	-	6
	$\gamma\text{-}Fe$	-0.15	-	-	10
<hr/>					
$Fe_{1000}/C_{PET}$	$\alpha\text{-}Fe$	0.0	0.0	33.0	49
	$Fe_3C$	0.15	0.02	21.0	38
	$\gamma\text{-}Fe(C)$	0.40	0.69	-	4
	$\gamma\text{-}Fe$	-0.13	-	-	9