

Electronic Supplementary Information

Reaction of Bisphenol A with Synthetic and Commercial $\text{MnO}_{x(s)}$: Spectroscopic and Kinetic Study

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Contents

Table S1. Summary of physical and chemical characteristics of MnO _x (s) media used in this study.	S3
Table S2. Mn 3s multiplet splitting results for a) Reference Mn oxides and b) control and reacted samples. Curve 1 and curve 2 corresponds to the position/binding energy of ⁵ S and ⁷ S for each sample.	S4
Table S3. Percentage composition of oxygen species obtained from fitting high resolution XPS O 1s spectra.	S5
Table S4. Percentage composition of carbon species obtained from fitting high resolution XPS C 1s spectra.	S6
Figure S1. Batch reactors (200mL) with corresponding reaction conditions used to for study of BPA removal with MnO _x (s).....	S7
Figure S2. Amount of BPA removed solely by adsorption onto (a) Syn-MnO _x and (b) Com-MnO _x . The maximum adsorbed amount was calculated by extrapolating the data to time=0.....	S8
Figure S3. Fitting of O 1s XPS high resolution spectra for replicate samples of (a) SynMnO _x Control (b) SynMnO _x Reacted (c) ComMnO _x Control and (d) ComMnO _x Reacted. The sample XPS spectra are shown as the black dashed lines; the solid green lines are the overall contribution due to fitting of different individual oxygen bonds.	S9
Figure S4. Fitting of C 1s XPS high resolution spectra for replicate samples of (a) SynMnO _x Control (b) SynMnO _x Reacted (c) ComMnO _x Control and (d) ComMnO _x Reacted. The sample XPS spectra are shown as the dashed black lines; the green solid lines are the overall contribution due to fitting of different individual carbon bonds.	S10

Table S1. Summary of physical and chemical characteristics of MnO_x(s) media used in this study.

	Com-MnO _x	Syn-MnO _x
Specific surface area (m²/g)	13.6	128.3
Elemental composition (%)		
Manganese	71.2	99.9 ^a
Aluminum	9.65	-
Iron	8.97	-
Silicon	6.88	-
Potassium	1.34	-
Titanium	0.425	-
Barium	0.367	-
Calcium	0.302	-

Specific surface area data from Multipoint – N₂ BET; Elemental composition data from X-ray Fluorescence (XRF); ^a data from SEM/EDS

a)

Table S2. Mn 3s multiplet splitting results for a) Reference Mn oxides and b) control and reacted samples. Curve 1 and curve 2 corresponds to the position/binding energy of ^{55}S and ^{75}S for each sample.

	Sample	Curve 1: Mn ^{55}S (eV)	Curve 2: Mn ^{75}S (eV)	Multiplet Splitting (eV)	Oxidation State
b) <u>References</u>	MnO; Mn(II)	89.10	83.40	5.69	2
	Mn ₂ O ₃ ; Mn(III)	88.52	83.20	5.33	3
	Li Mn(III,IV)O	88.94	84.05	4.90	3.5
	MnO ₂ ; Mn(IV)	88.89	84.52	4.38	4
<u>Samples</u>	Syn-MnO _x Control	89.40	84.77	4.63	3.7
	Syn-MnO _x Reacted	89.27	84.45	4.82	3.4
	Com-MnO _x Control	87.04	82.57	4.47	3.9
	Com-MnO _x Reacted	87.93	83.25	4.68	3.7

Table S3. Percentage composition of oxygen species obtained from fitting high resolution XPS O 1s spectra. Uncertainty shown is standard deviation for triplicate data.

BE->	529.6	531.2	532.5	533.7	535.0
	MnOx	O=N-C/ C=O	-C-OH	C-O-C / COOH	C-O-O-C
Syn-MnOx Control	59.4 ± 3.8	19.4 ± 1.3	13.3 ± 1.2	7.9 ± 1.3	0.0
Syn-MnOx Reacted	33.0 ± 1.4	23.3 ± 0.5	20.7 ± 0.1	17.7 ± 0.7	5.3 ± 0.6
Com-MnOx Control	17.2 ± 1.5	19.8 ± 0.2	28.4 ± 1.7	22.1 ± 1.3	12.5 ± 1.3
Com-MnOx Reacted	13.7 ± 0.4	14.0 ± 6.1	20.6 ± 4.1	30.0 ± 2.6	21.6 ± 8.0

Table S4. Percentage composition of carbon species obtained from fitting high resolution XPS C 1s spectra. Uncertainty shown is standard deviation for triplicate data.

Binding Energy (eV) ->	284.7	285.6	287.2	288.5
	C-C/C=C	C*-C-Ox	C-OH	C=O
Syn-MnOx Control	65.2 ± 3.3	4.4 ± 1.1	21.2 ± 3.1	9.2 ± 1.4
Syn-MnOx Reacted	63.4 ± 2.2	0.4 ± 0.3	26.6 ± 0.8	9.7 ± 1.6
Com-MnOx Control	34.7 ± 6.1	3.2 ± 0.3	33.0 ± 4.0	29.1 ± 9.7
Com-MnOx Reacted	26.4 ± 8.4	1.2 ± 0.04	40.9 ± 5.7	31.5 ± 2.6

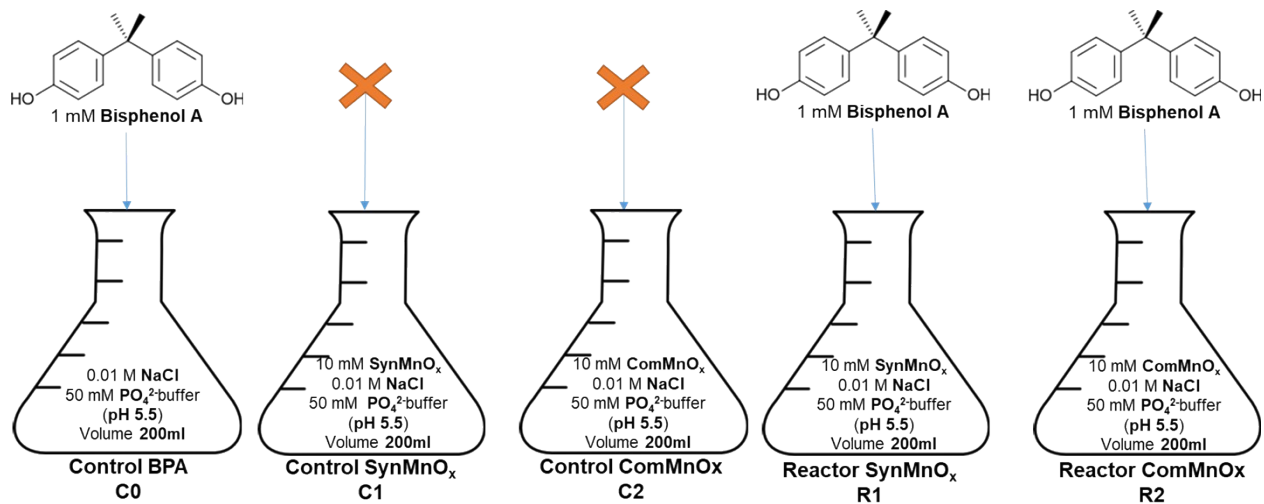


Figure S1. Batch reactors (200mL) with corresponding reaction conditions used to for study of BPA removal with MnO_x(s).

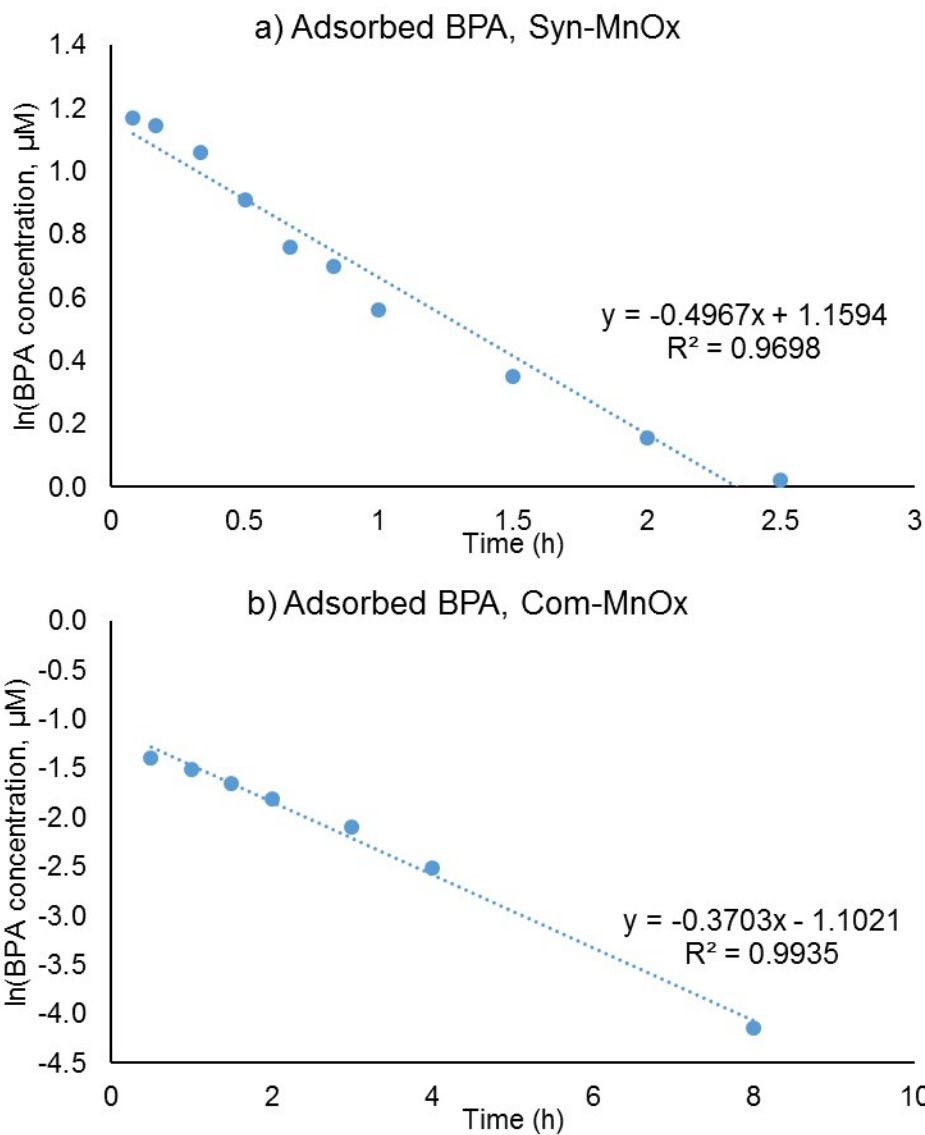


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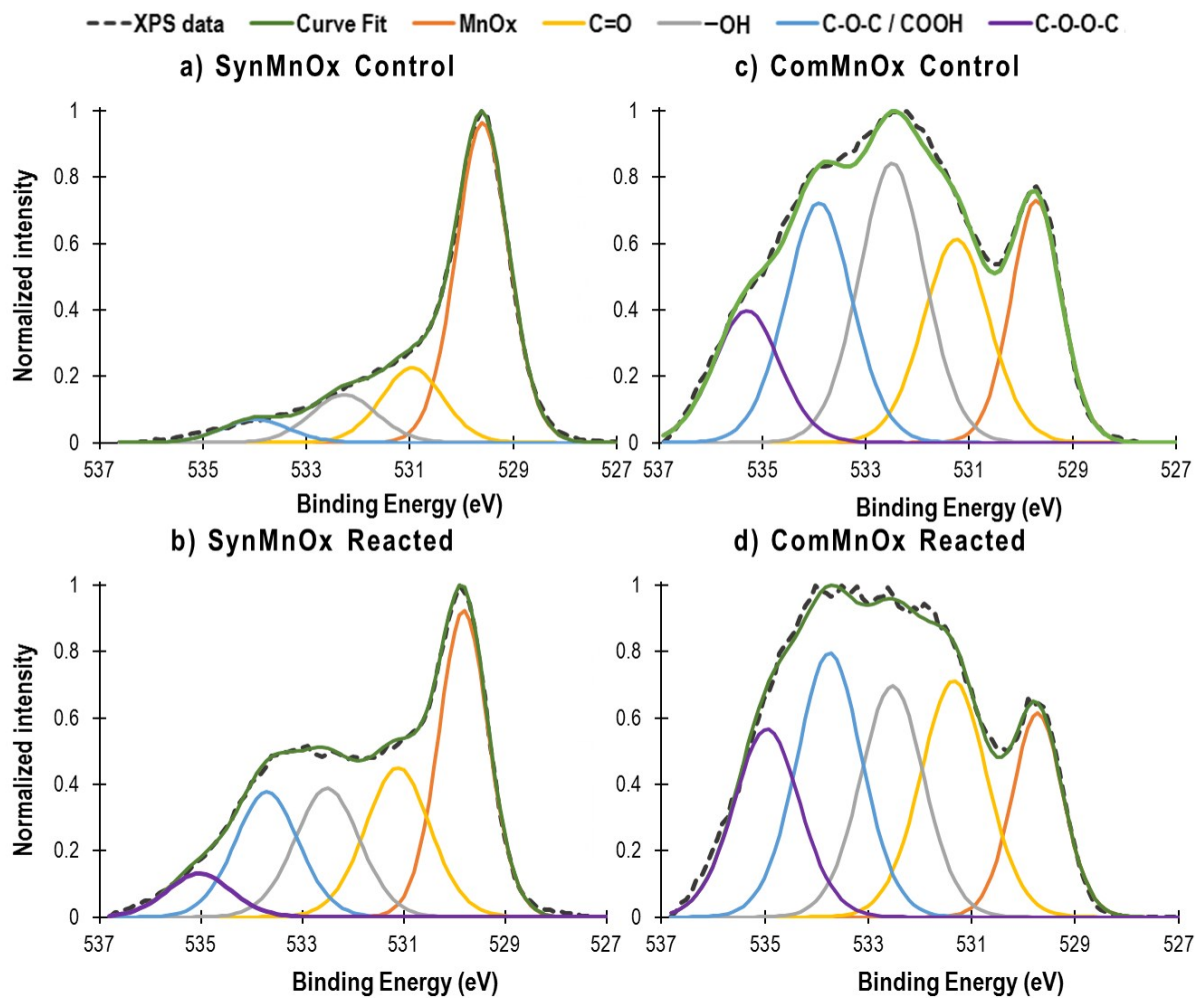


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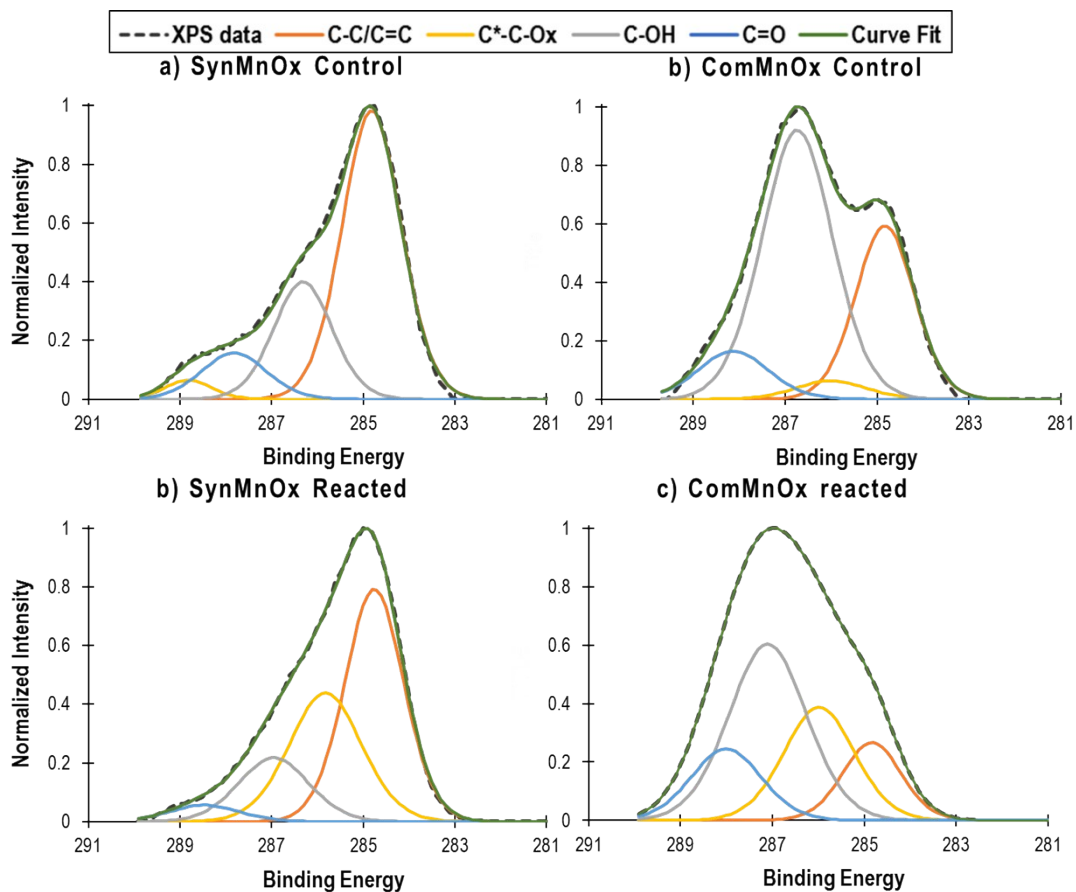


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