

Supporting Information for:

Circular Design and Functionalized Upcycling of Waste Commodity Polystyrene via C-H Activation Using Microwave-Assisted Multicomponent Synthesis

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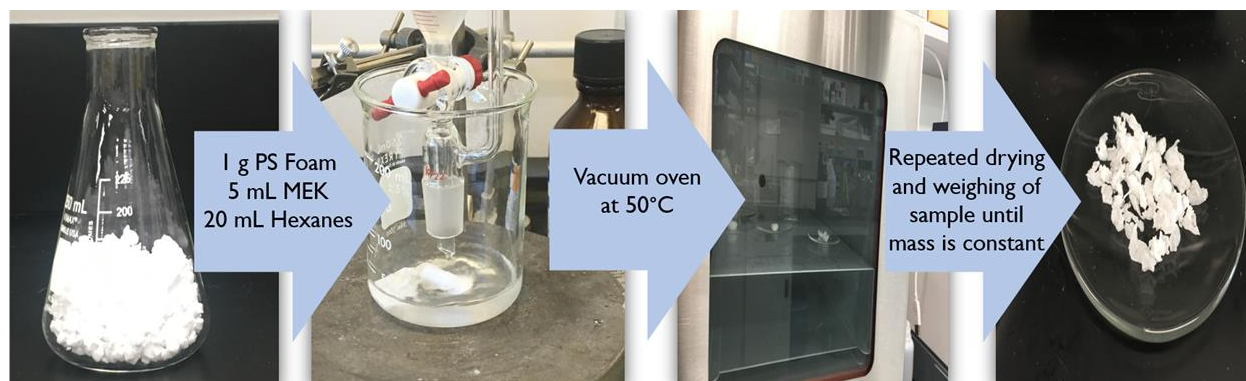


Figure S1. The optimized procedure for recovery of polystyrene from waste clamshell containers.

Table S1: Optimization of the dissolution/precipitation method (n=3)

Polystyrene (g)	MEK (mL)	Hexanes (mL)	MEK:Hexanes Ratio	Recovered Yield (%)
Dissolution/Precipitation Method				
1.00	5.00	20	1:4	81.4 ± 0.06
1.00	5.00	50	1:10	75.2 ± 0.43
1.00	5.00	100	1:20	82.3 ± 0.01
Reverse Precipitation Method				
1.00	5.00	50	1:10	77.9 ± 0.12
1.00	5.00	35	1:7	98.5 ± 0.003
1.00	5.00	25	1:5	99.5 ± 0.037
1.00	5.00	20	1:4	102
1.00	5.00	16.5	1:3.3	99.1 ± 0.006
1.00	5.00	15	1:3	98.5 ± 0.002



Image I1: Rutile and anatase mixed phases in the Fe/TiO₂ catalyst.

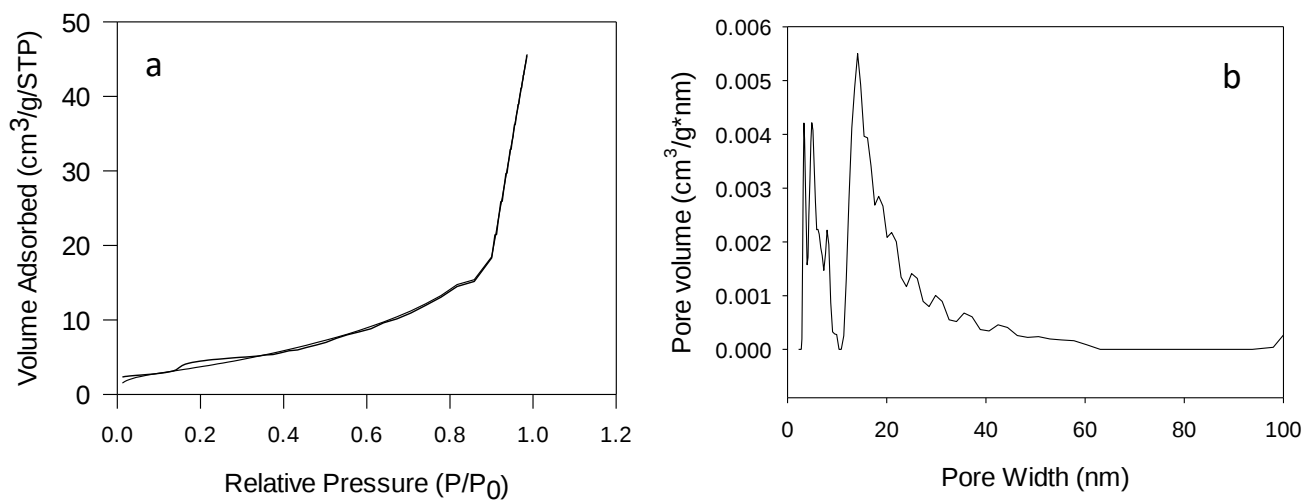


Figure S2. (a) N₂ adsorption isotherm of Fe/TiO₂ and (b) Fe/SiO₂ along with corresponding pore size distribution derived from adsorption isotherm (inset)

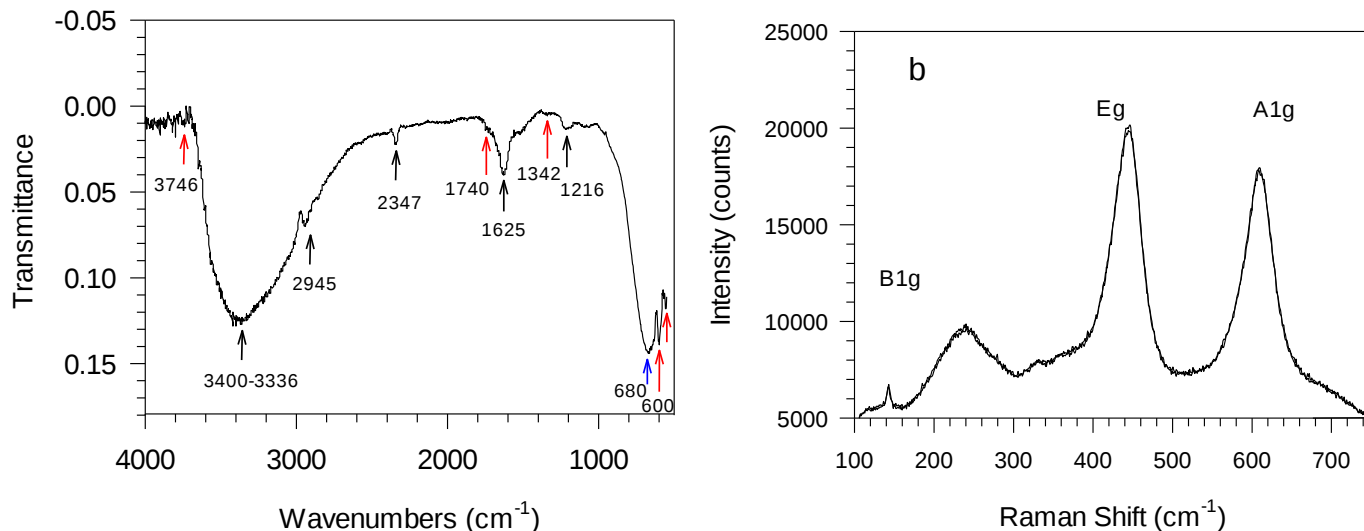


Figure S3. (a) FTIR spectrum of the Fe/TiO₂ catalyst. The red arrows indicate the characteristic peaks for anatase phase, and the blue arrows indicates the characteristic peaks for the rutile phase. (b) Raman Spectrum for the red specs in the catalyst to show the rutile phase.

Table S2: FTIR peak assignments for the mixed anatase and rutile phases of Fe/TiO₂ catalyst.

Peaks (cm ⁻¹)	Assignment	Phase		Reference
		Anatase	Rutile	
549	Ti-O	+	-	[1]
600	Ti-O	+	-	[1]
680	Ti-O-Ti	-	+	[1]
1216	C-O	+	+	
1625	O-H bending of molecularly adsorbed H ₂ O	+	+	[2]
1740	Titanium carboxylates	+	-	[1,3]
2945	C-H	+	+	
3366	Ti-OH stretching	+	+	[1,3]
3400	O-H stretching	+	+	[1-3]
3746	Free O-H	+	-	[2,3]

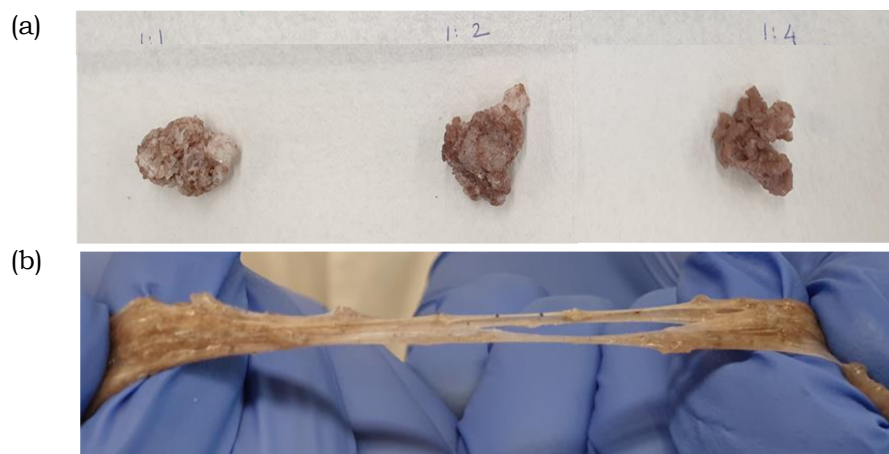


Figure S4. (a) Integration of F:M ratios with recovered PS and (b) adhesive nature of MPS4

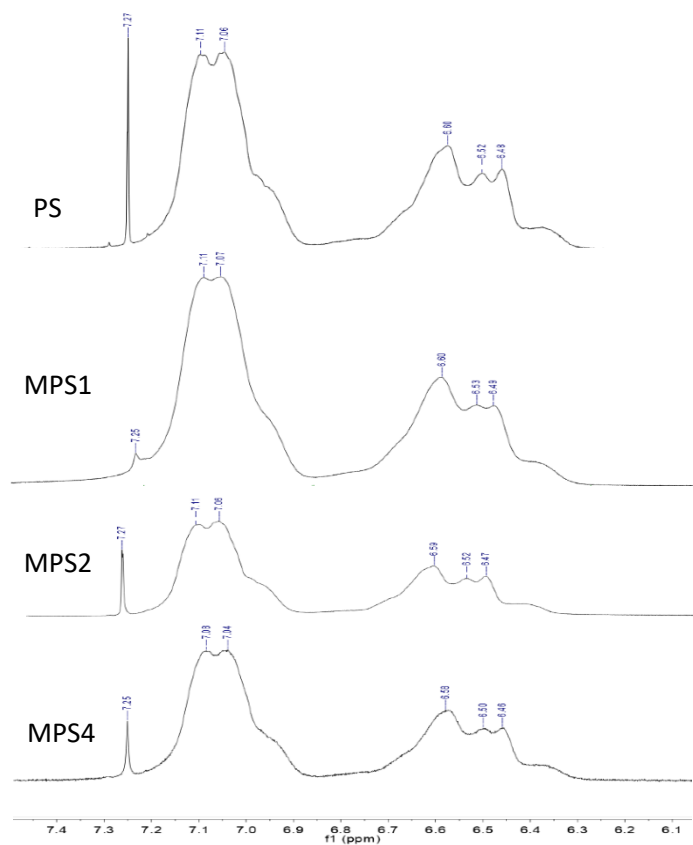


Figure S5: ^1H NMR chemical shifts and J-values for the aromatic region of PS and the various ratios of the functionalized polymers

Table S3: XPS data for the C1s, N1s and O1s of the functionalized polystyrene ratios

	MPS1		MPS2		MPS4	
	Binding Energy (e.V)	Atomic (%)	Binding Energy (e.V)	Atomic (%)	Binding Energy (e.V)	Atomic (%)
C1s						
C-C, C-H	284.91	96.99	284.93	93.60	284.94	82.22
C=N/C-N/C-O	286.63	0.80	286.62	1.79	286.64	4.41
C=O	287.73	0.83	287.30	1.37	287.74	2.35
<i>C1s total:</i>		<i>98.62</i>		<i>96.76</i>		<i>88.98</i>
N1s						
N=C/C=N	397.30	0.00069	397.20	0.00	397.28	0.0547
N-C, N-C=O	399.89	0.23	399.80	1.04	399.88	2.56
-NH ₃ ⁺	402.10	0.20	402.00	0.252	402.08	0.138
<i>N1s total:</i>		<i>0.43</i>		<i>1.29</i>		<i>2.75</i>
O1s						
O-(C=O), O=C aliphatic	532.40	0.087	531.80	0.359	531.10	0.355
O-C (aliphatic)	532.85	0.085	532.89	1.56	532.45	7.92
<i>O1s total:</i>		<i>0.17</i>		<i>1.92</i>		<i>8.28</i>

REFERENCES

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