Silane functionalization of WS2 Nanotubes for interaction with Poly(lactic acid)

Supplementary information

FTIR

Table S1. FTIR tabulated Peak wavenumber assignment of APTES in comparison to WS_2-APTES samples.

Peak Wavenumber cm^{-1}	**Neat APTES**	**Peak Wavenumber cm^{-1}**	**WS_2 APTES**
3383 2974	NH_2 stretching	3348 3270	N-H vibrations
2927 2883	Asymmetric CH Symmetric CH	2925 2860	Asymmetric CH Symmetric CH
1604 1483	NH_2 deformation bending	1628 1570 1470	scissor modes of $-NH_2$ (shoulder) asymmetric $-NH_3^+$ symmetric $-NH_3^+$
1442 1390	O-H bending	1383	O-H bending
1294 1165	C-O stretching	1232 1191	$Si-CH_2-CH_2$ C-O stretching
1073 765	Asymmetric Si-O-Si Symmetric Si-O-Si	1108 (WS_2: APTES1:1) 1100 (WS_2: APTES1:2) 1092 (WS_2:APTES1:4) 745	Asymmetric Si-O-Si Symmetric Si-O-Si
1100	Si-O-C asymmetric	1012 (WS_2: APTES1:1) 1005 (WS_2: APTES1:2) 999 (WS_2: APTES 1:4)	Si-O-C asymmetric
954 853	Si-OH stretching Si-OH bending	933 (WS_2: APTES 1:1) 929 (WS_2: APTES 1:2) 925 (WS_2: APTES 1:4) 858	Si-OH stretching Si-OH bending
677	N-H bending	690	N-H bending

XPS Deconvoluted graphs and corresponding atomic percentages

Table S2. WS_2 NTs XPS deconvoluted data

O 1s region		
Binding energy (eV)	% of region	Bonding environment
530.94	6.6	WO_3
532.28	71.8	O-C
533.61	21.6	O*-(C=O)
C 1s region		
Binding energy (eV)	% of region	Bonding environment
284.09	48.6	C-C/C-H
285.45	41.8	C-O
286.98	4.1	C=O
289.23	5.5	O=C-O
S 2p region		
Binding energy (eV)	% of region	Bonding environment
162.38	50.0	S $2p_{3/2}$ - WS_2
163.56	50.0	S $2p_{1/2}$ - WS_2
W 4f & W 5p3/2 region		
Binding energy (eV)	% of region	Bonding environment
32.75	35.6	W $4f_{7/2}$ - WS_2
34.89	34.0	W $4f_{5/2}$ - WS_2
36.05	3.0	W $4f_{7/2}$ - WO_3
38.19	2.9	W $4f_{5/2}$ - WO_3
38.56	24.5	W $5p_{3/2}$

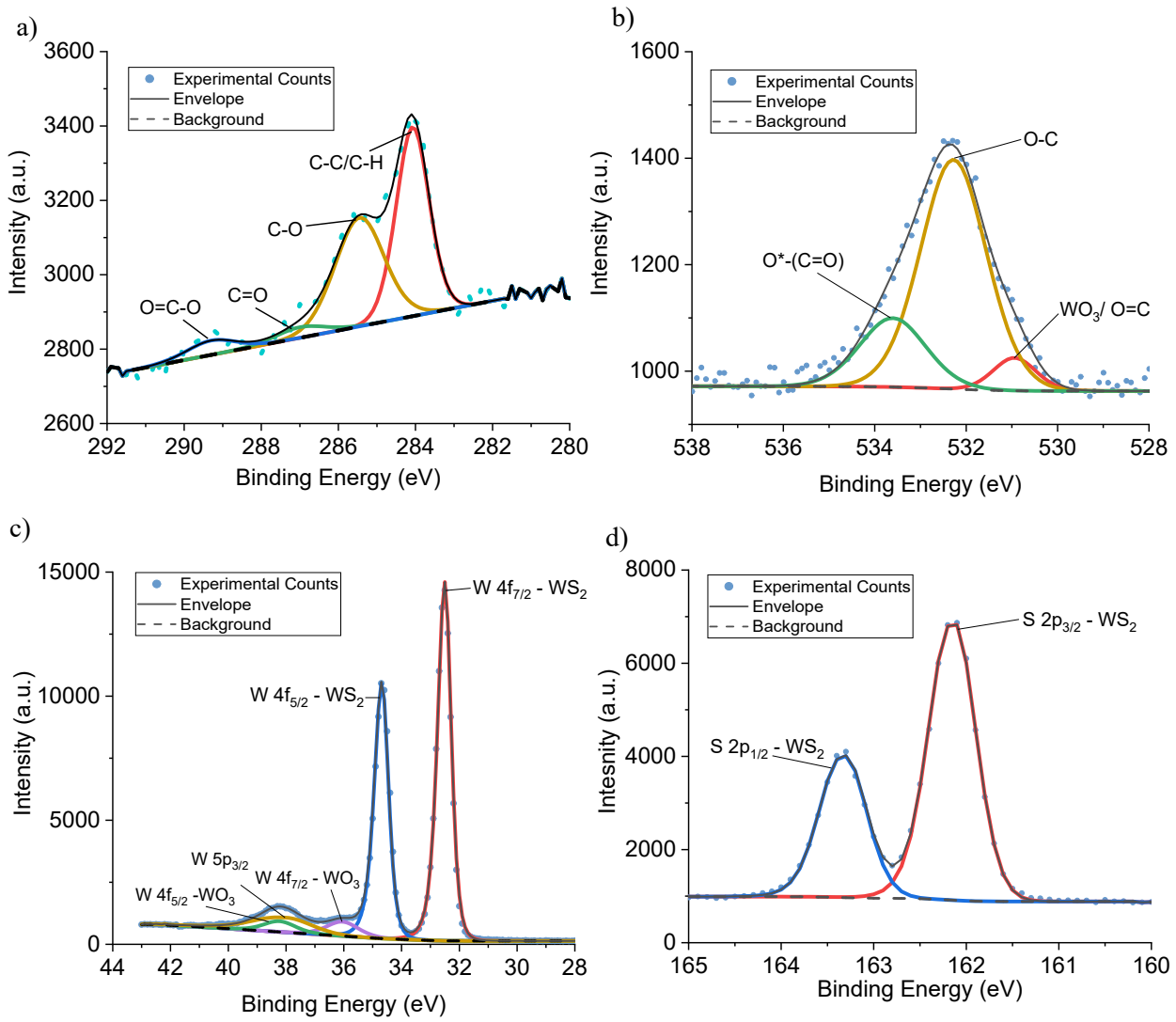

Figure S1. Deconvoluted XPS spectra a) C1s ,b) O 1s ,c) W 4f 1:2, d)Si 2p, regions of XPS spectra for WS_2 NTs sample

Table 3. WS_2 NTs- APTES 1:1 XPS deconvoluted data

C 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
285	59.2	C-C/C-H
286.19	16.3	C-O
287.74	2.3	C=O
288.8	2.7	O=C-O
285.72	19.5	C-N
O 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
531.17	8.5	O=C / WO_3
532.51	87.3	O-C / O-Si
534.11	4.2	O*-(C=O)
N 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
399.54	90.8	N-C (APTES)
401.14	9.2	NR4+
Si 2p region		
Binding energy (eV)	**% of region**	**Bonding environment**
102.6	50.5	Si $2p_{3/2}$
103.21	49.5	Si $2p_{1/2}$
S 2s region		
Binding energy (eV)	**% of region**	**Bonding environment**
226.29	100	WS_2
W 4f region		
Binding energy (eV)	**% of region**	**Bonding environment**
32.43	29.6	W $4f_{7/2}$ - WS_2
34.59	28.3	W $4f_{5/2}$ - WS_2
38.28	29.0	W $5p_{3/2}$
35.2	6.7	W $4f_{7/2}$ - WO_3
37.36	6.4	W $4f_{5/2}$ - WO_3

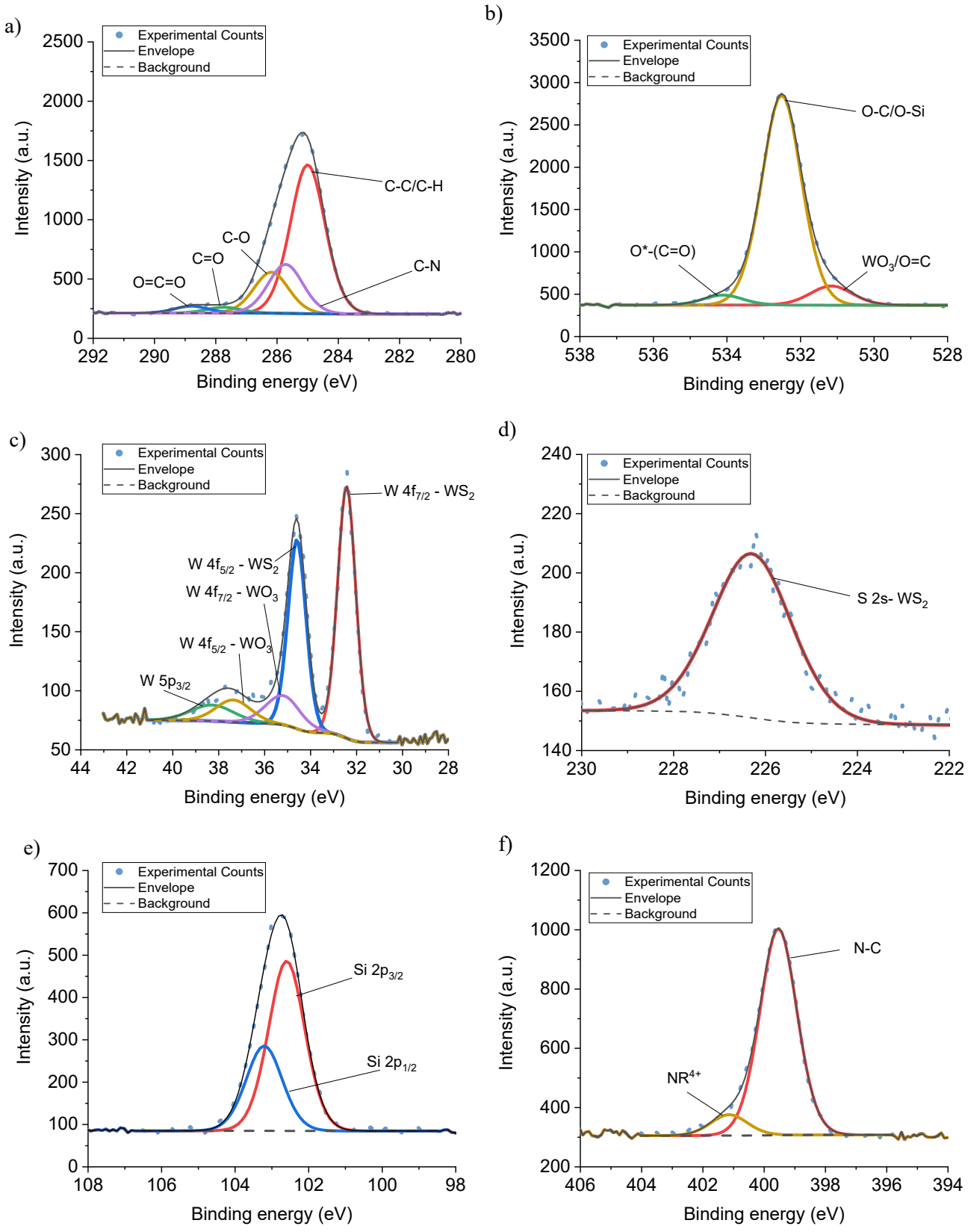

Figure S2. Deconvoluted XPS spectra a) C1s b) O 1s c) W 4f 1:2, d)Si 2p, e)N 1s f)S 2s regions of XPS spectra for WS_2-APTES 1:1 sample

Table 4. WS_2 NTs- APTES 1:2 XPS deconvoluted data

C 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
285	68.3	C-C/C-H
286.44	14.0	C-O
287.74	0.4	C=O
288.8	8.9	O=C-O
285.7	8.4	C-N
O 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
530.54	2.3	O=C / WO_3
532.34	79.4	O-C / O-Si
533.55	18.3	O*-(C=O)
N 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
399.51	90.8	N-C (APTES)
401.12	9.2	NR4+
Si 2p region		
Binding energy (eV)	**% of region**	**Bonding environment**
102.48	50.5	Si $2p_{3/2}$
103.09	49.5	Si $2p_{1/2}$
S 2s region		
Binding energy (eV)	**% of region**	**Bonding environment**
226.24	100	WS_2
W 4f region		
Binding energy (eV)	**% of region**	**Bonding environment**
32.28	31.8	W $4f_{7/2}$ - WS_2
34.44	30.3	W $4f_{5/2}$ - WS_2
38.13	31.2	W $5p_{3/2}$
35.05	3.4	W $4f_{7/2}$ - WO_3
37.21	3.3	W $4f_{5/2}$ - WO_3

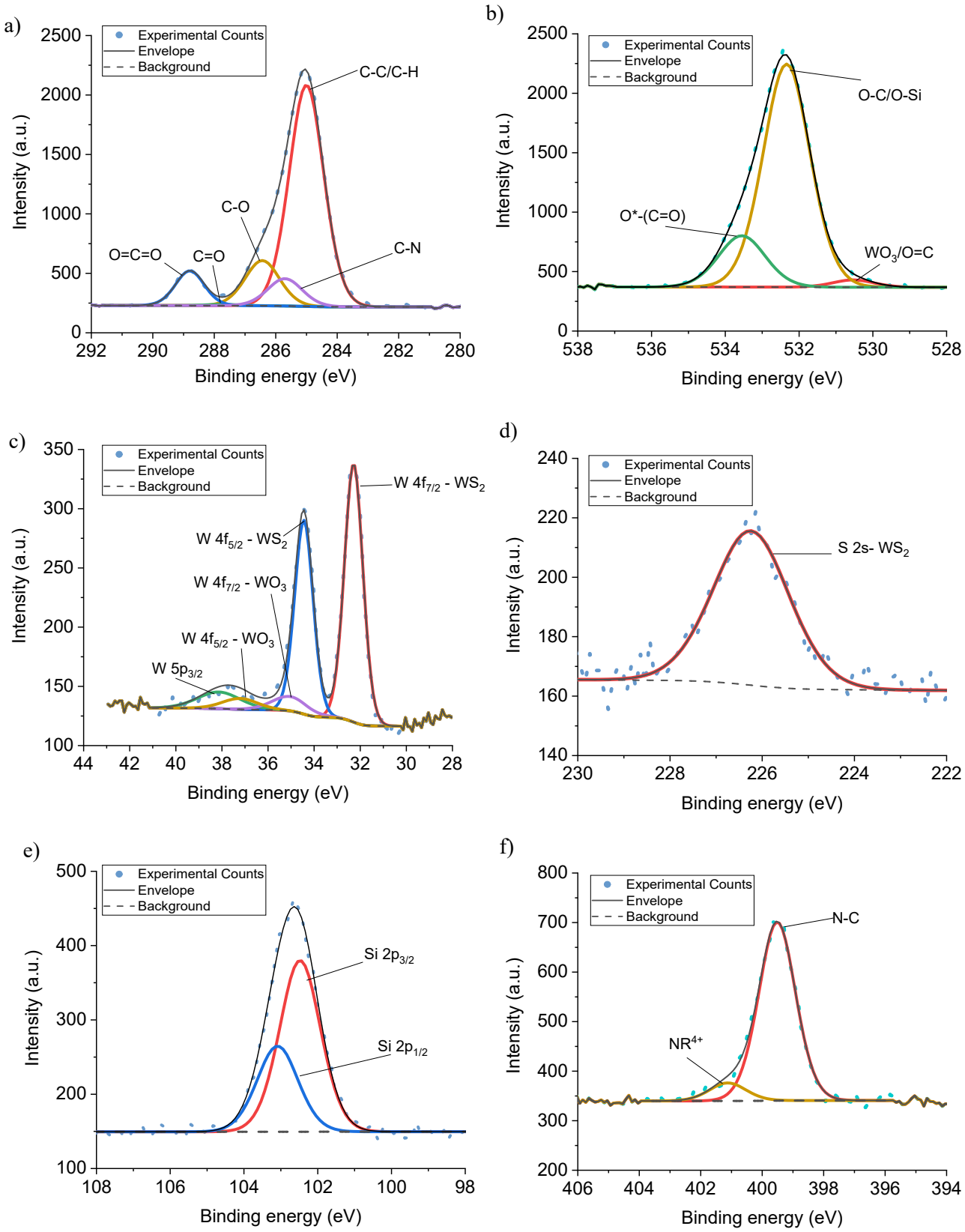

Figure S3 Deconvoluted XPS spectra a) C1s b) O 1s c) W 4f 1:2, d)Si 2p, e)N 1s f)S 2s regions of XPS spectra for WS_2-APTES 1:2 sample

Table 5.WS2 NTs- APTES 1:4 XPS deconvoluted data

C 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
285	69.0	C-C/C-H
286.44	10.8	C-O
287.74	1.2	C=O
288.8	6.7	O=C-O
285.7	12.3	C-N
O 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
530.82	3.8	O=C / WO_3
532.35	83.8	O-C / O-Si
533.56	12.4	O*-(C=O)
N 1s region		
Binding energy (eV)	**% of region**	**Bonding environment**
399.42	81.3	N-C (APTES)
401.03	8.3	NR4+
396.66	10.4	W-N
Si 2p region		
Binding energy (eV)	**% of region**	**Bonding environment**
102.44	50.5	Si $2p_{3/2}$
103.05	49.5	Si $2p_{1/2}$
S 2s region		
Binding energy (eV)	**% of region**	**Bonding environment**
226.2	100	WS_2
W 4f region		
Binding energy (eV)	**% of region**	**Bonding environment**
32.3	31.9	W $4f_{7/2}$ - WS_2
34.46	30.4	W $4f_{5/2}$ - WS_2
38.15	31.3	W $5p_{3/2}$
35.07	3.3	W $4f_{7/2}$ - WO_3
37.23	3.1	W $4f_{5/2}$ - WO_3

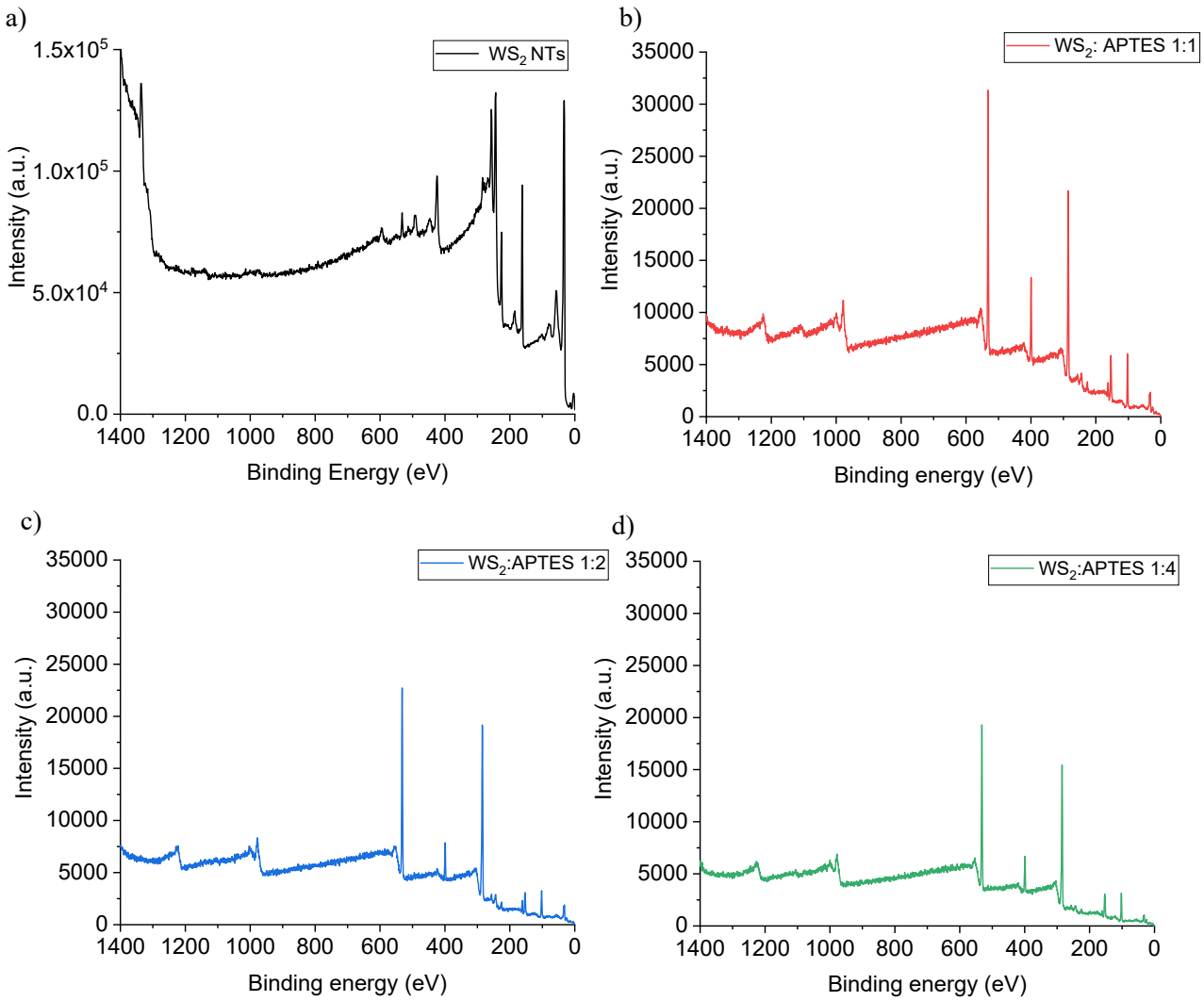

Figure S4. Survey XPS spectra a) WS_2 NTs b) WS_2:APTES 1:1 c) WS_2:APTES 1:2, d) WS_2:APTES 1:4