Electronic Supplementary Material (ESI) for Nanoscale.

CO_2 controlled flocculation of microalgae using pH responsive cellulose nanocrystals - Supplementary Information

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S1 FTIR Spectrscopy

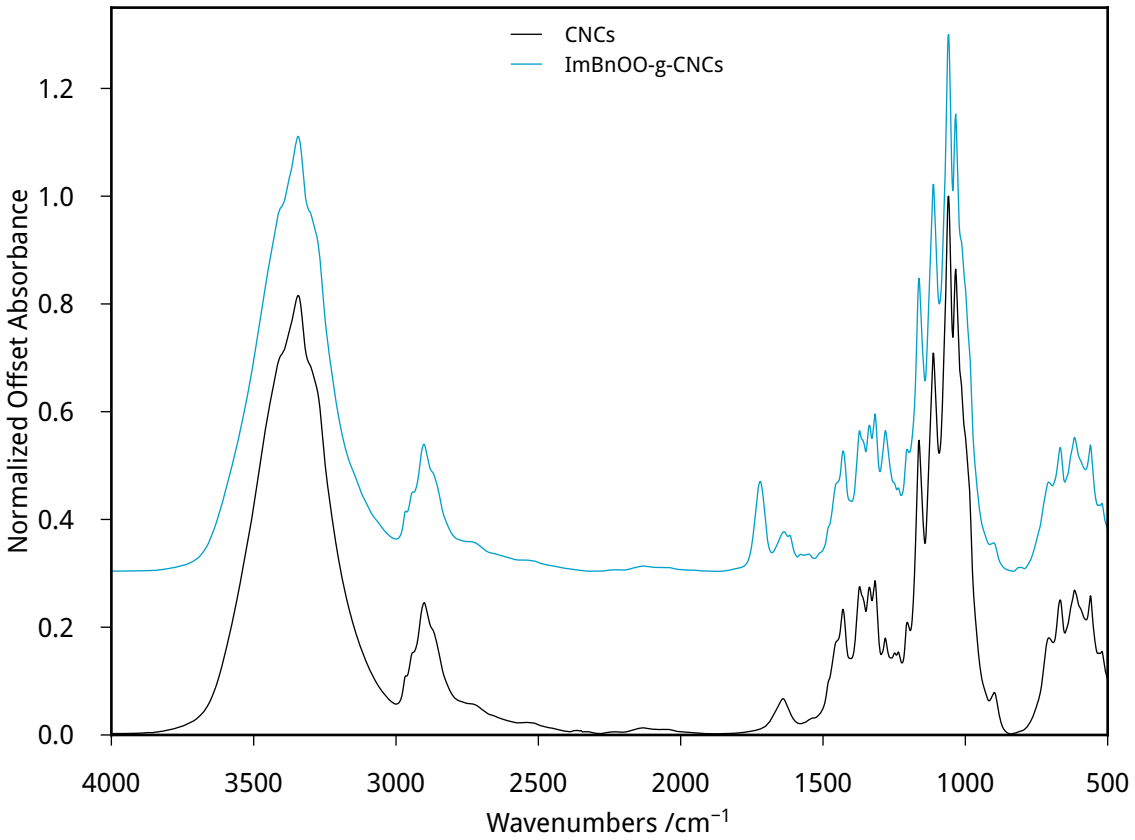

Fig. S1.1 FTIR spectra of modified CNCs displayed as offset absorbance spectra

S2 TGA

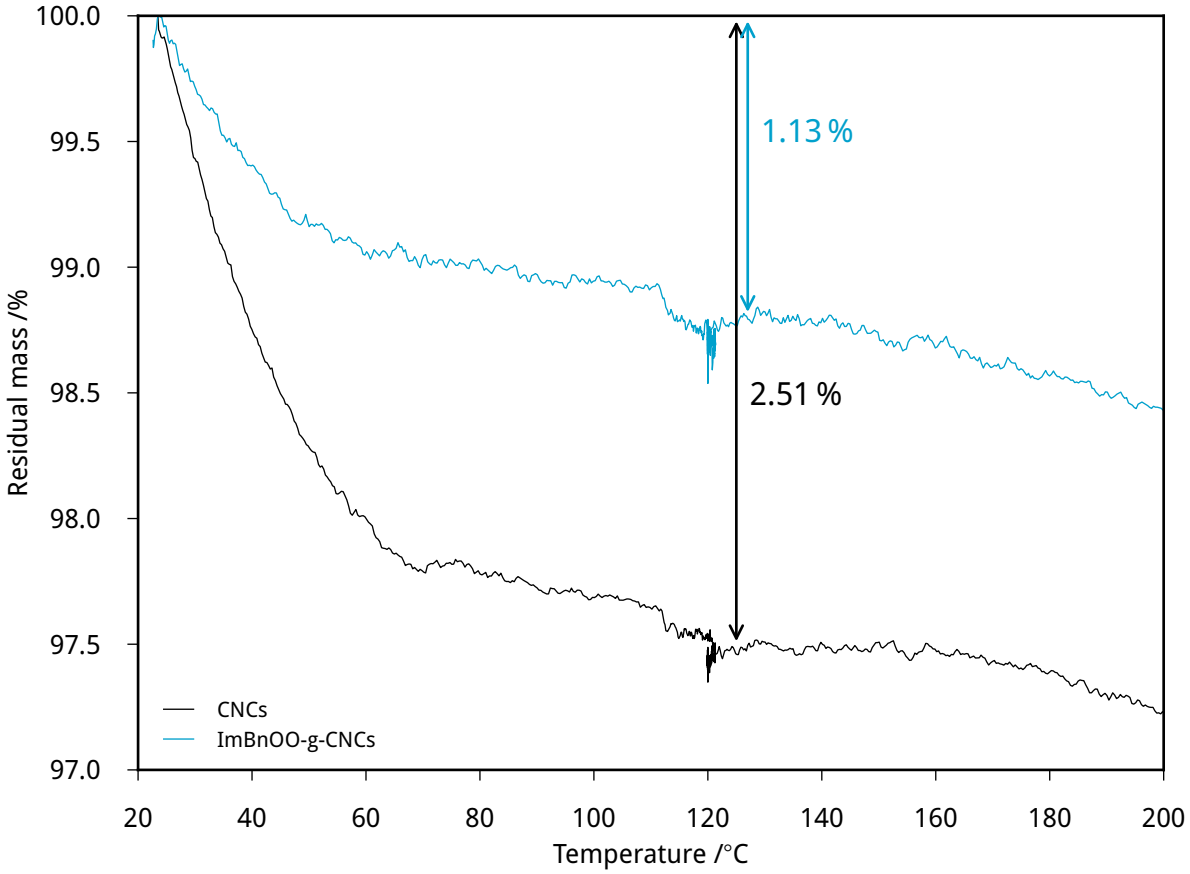

Fig. S2.1 TGA data for CNCs and ImBnOO-g-CNCs showing mass loss due to bound water at 125 °C.

S3 X-ray photoelectron spectroscopy

S3.1 Tables

Table S3.1 Table of XPS data for CNCs

Orbital	Component	Binding Energy /eV	FWHM /eV	Rel. A /%[a]	At %
C 1s	C–C	285.0	1.1	7.78	4.74
	C–O	286.6	1.1	77.47	47.22
	O–C–O	288.3	1.1	14.75	8.99
	All			100	60.95
O 1s	C–O–H	532.7	1.2	60[b]	23.39
	O–C–O	533.3	1.2	40[b]	15.60
	All			100	38.99
S 2p[c]	$j = 3/2$	169.4	1.8	66.25	0.04
	$j = 1/2$	171.1	1.8	33.75	0.02
	All			100	0.06

[a] Area relative to other components of same orbital
[b] Fixed to reflect stoichiometry
[c] Rel. A/separation fixed to reflect spin-orbit splitting [1]

Table S3.2 Table of XPS data for ImBnOO-g-CNCs

Orbital	Component	Binding Energy /eV	FWHM /eV	Rel. A /%[a]	At %
C 1s	C–C	285.0	1.1	15.81	10.09
	C–O	286.5	1.1	69.66	44.44
	O–C–O	288.2	1.1	12.93	8.25
	O–C=O	289.6	1.1	1.60	1.02
	All			100	63.80
O 1s	C–O–H	532.6	1.3	59.89[b]	20.98
	O–C–O	533.2	1.3	40.11[b]	14.05
	All			100	35.03
N 1s[c]	Imidazole N 1	399.1	1.4	24.69	0.17
	Imidazole N 2	400.8	1.4	24.66	0.17
	Imidazolium N	402.0	1.4	50.65	0.34
	All			100	0.68
S 2p[d]	$j = 3/2$	168.6	1.4	66.25	0.11
	$j = 1/2$	170.2	1.4	33.75	0.05
	All			100	0.16
Cl 2p	$j = 3/2$	200.6	1.2	64.61	0.18
	$j = 1/2$	202.4	1.2	35.39	0.10
	All			100	0.28
Br 3d[d]	$j = 5/2$ Env. 1	68.1	1.0	36.84	0.02
	$j = 3/2$ Env. 1	69.1	1.0	24.54	0.01
	$j = 5/2$ Env. 2	70.7	1.0	23.18	0.01
	$j = 3/2$ Env. 2	71.7	1.0	15.44	0.01
	All			100	0.06

[a] Area relative to other components of same orbital
[b] Fixed to reflect stoichiometry
[c] Imidazole separation fixed based on Nolting et al.[2]
[d] Rel. A/separation fixed to reflect spin-orbit splitting[1,3]

S3.2 Wide scans

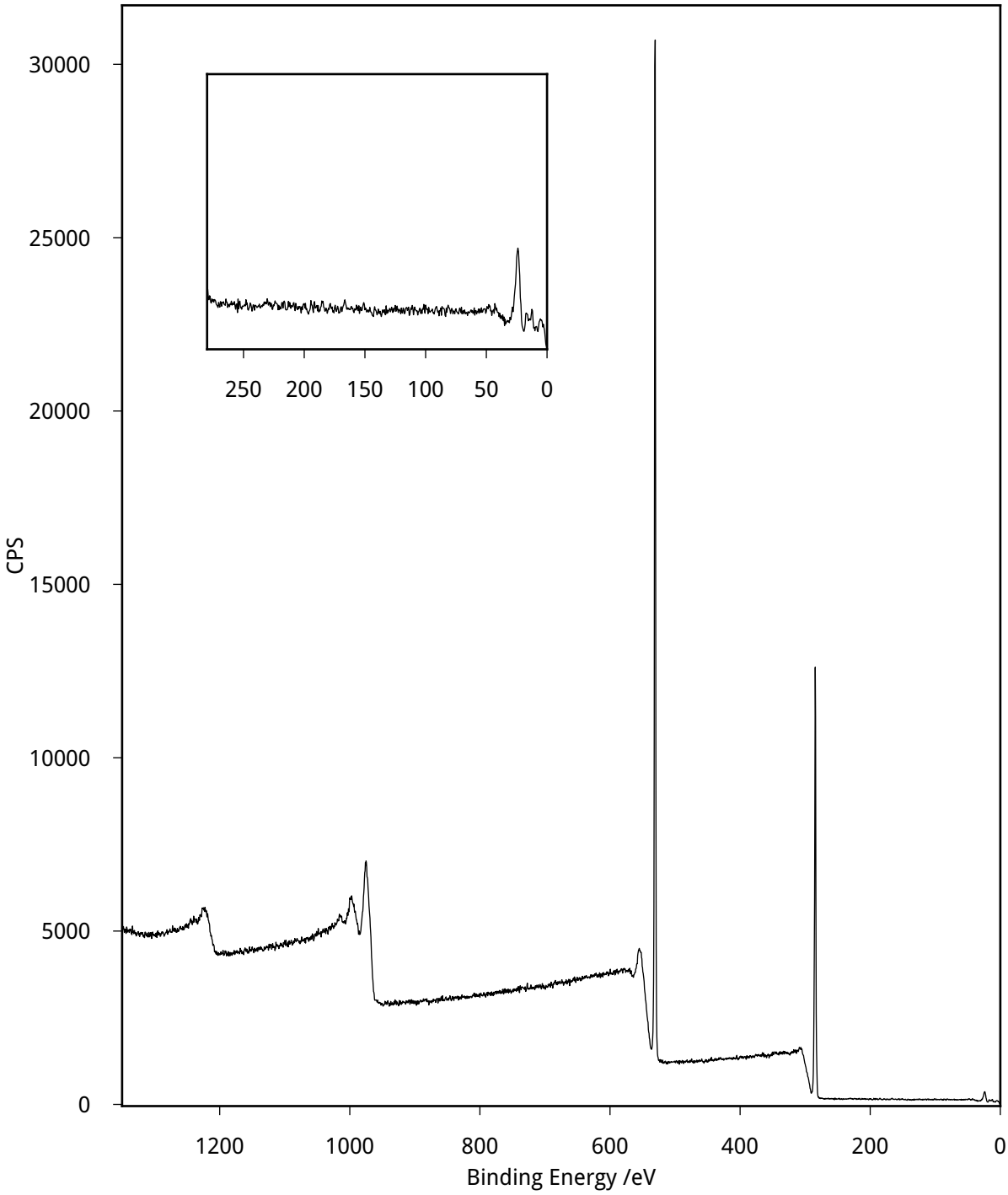

Fig. S3.1 XPS wide scan of CNCs

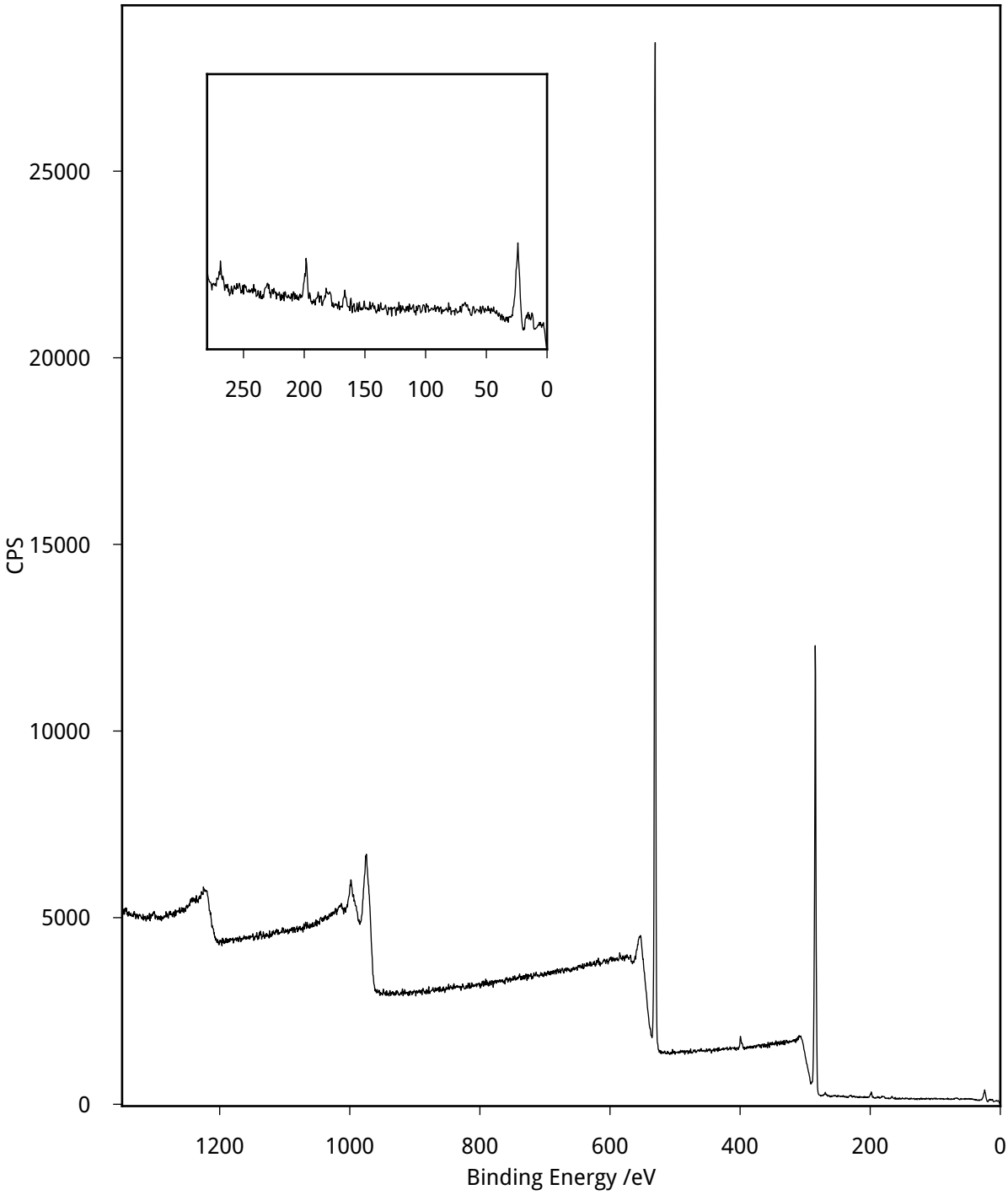

Fig. S3.2 XPS wide scan of ImBnOO-g-CNCs

S3.3 Carbon 1s scans

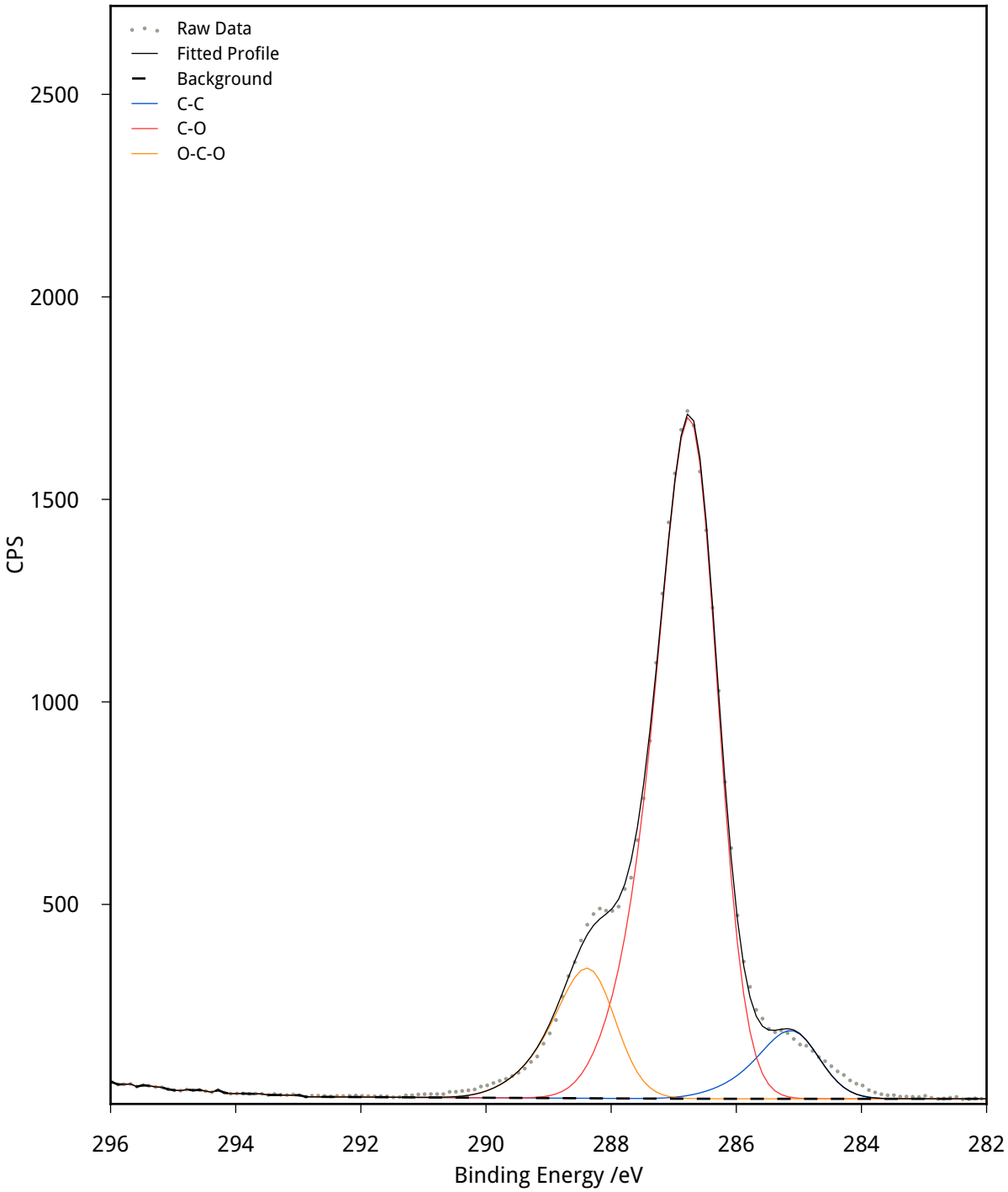

Fig. S3.3 XPS carbon 1s high resolution scan of CNCs

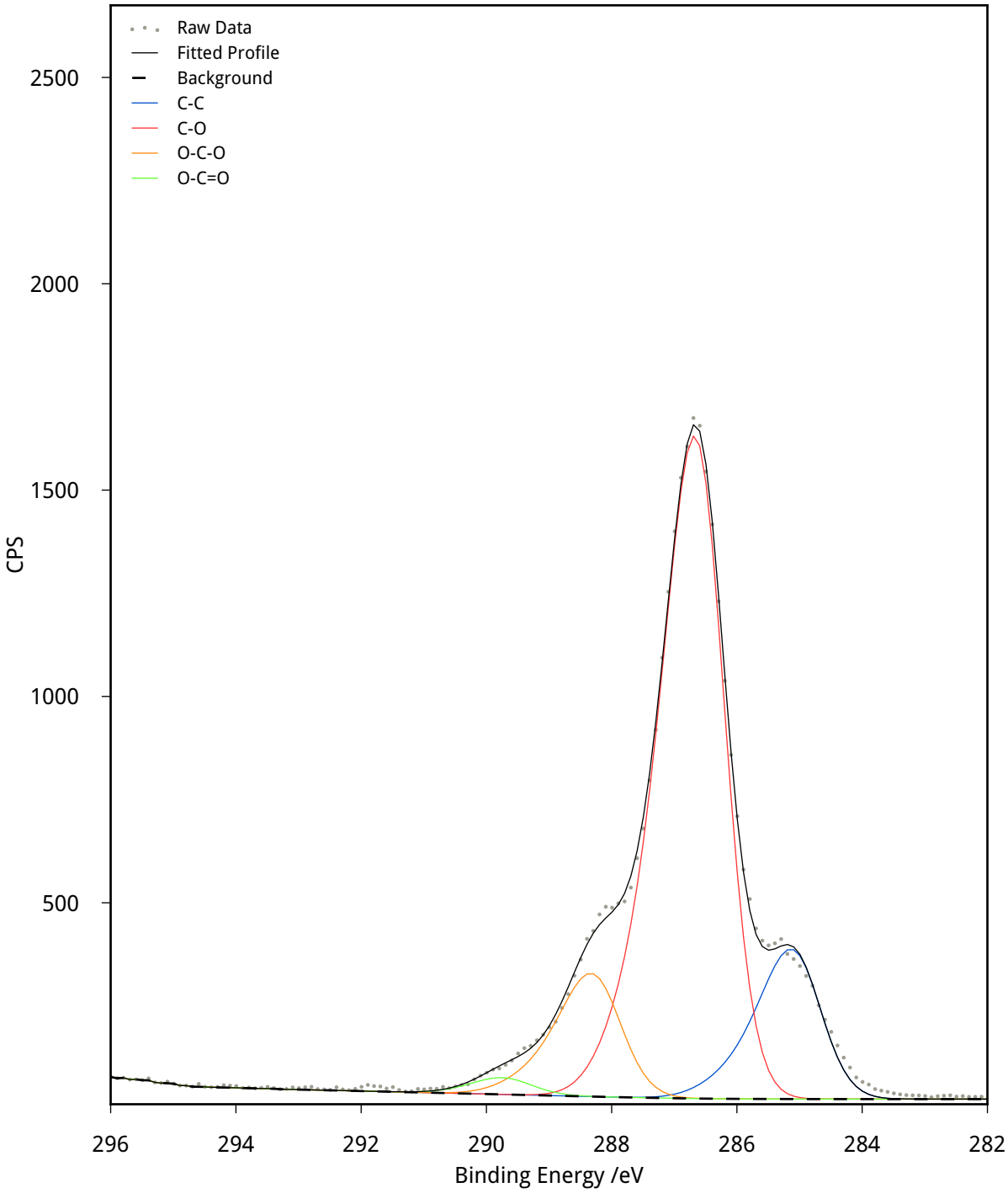

Fig. S3.4 XPS carbon 1s high resolution scan of ImBnOO-g-CNCs

S3.4 Oxygen 1s scans

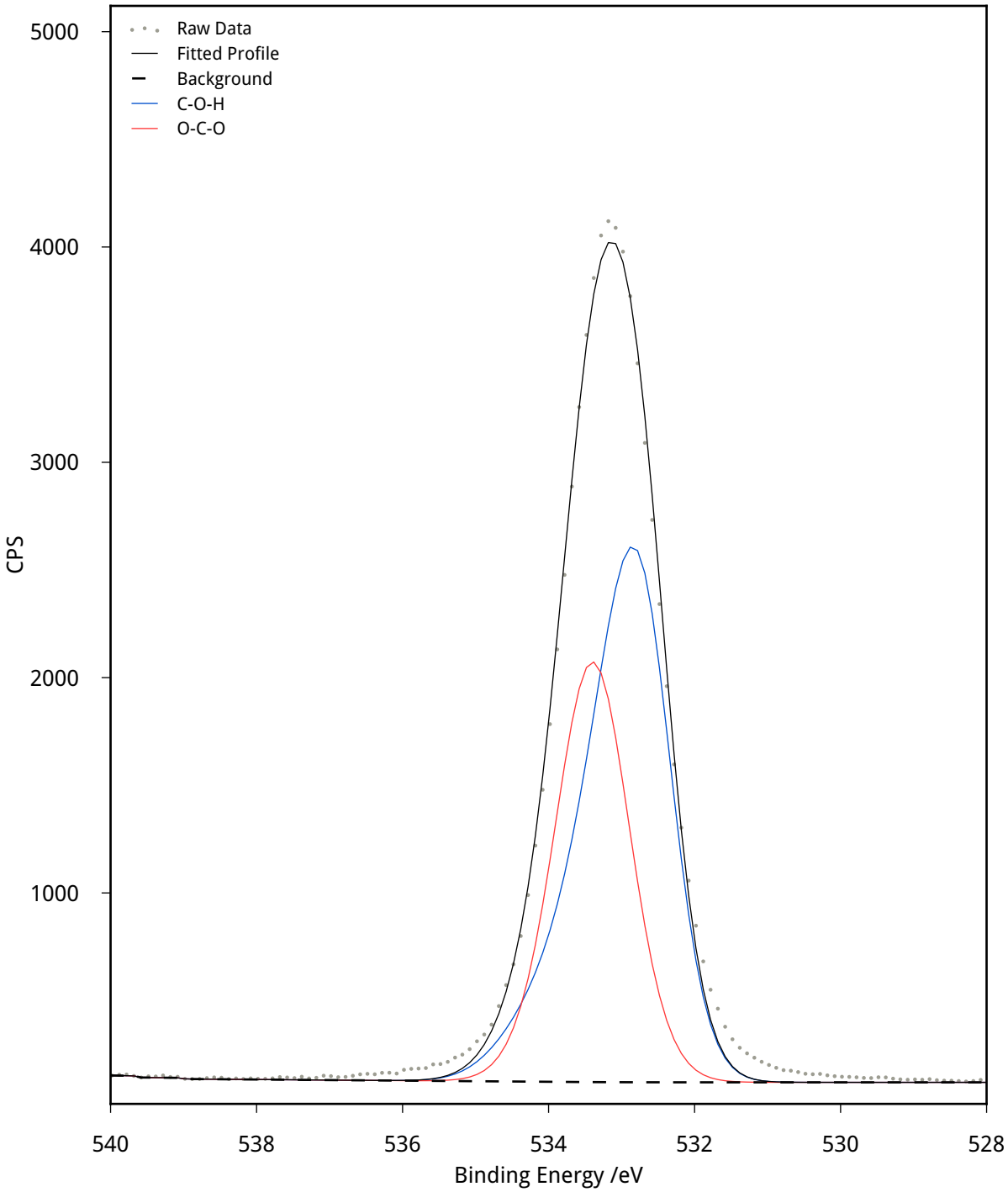

Fig. S3.5 XPS oxygen 1s high resolution scan of CNCs

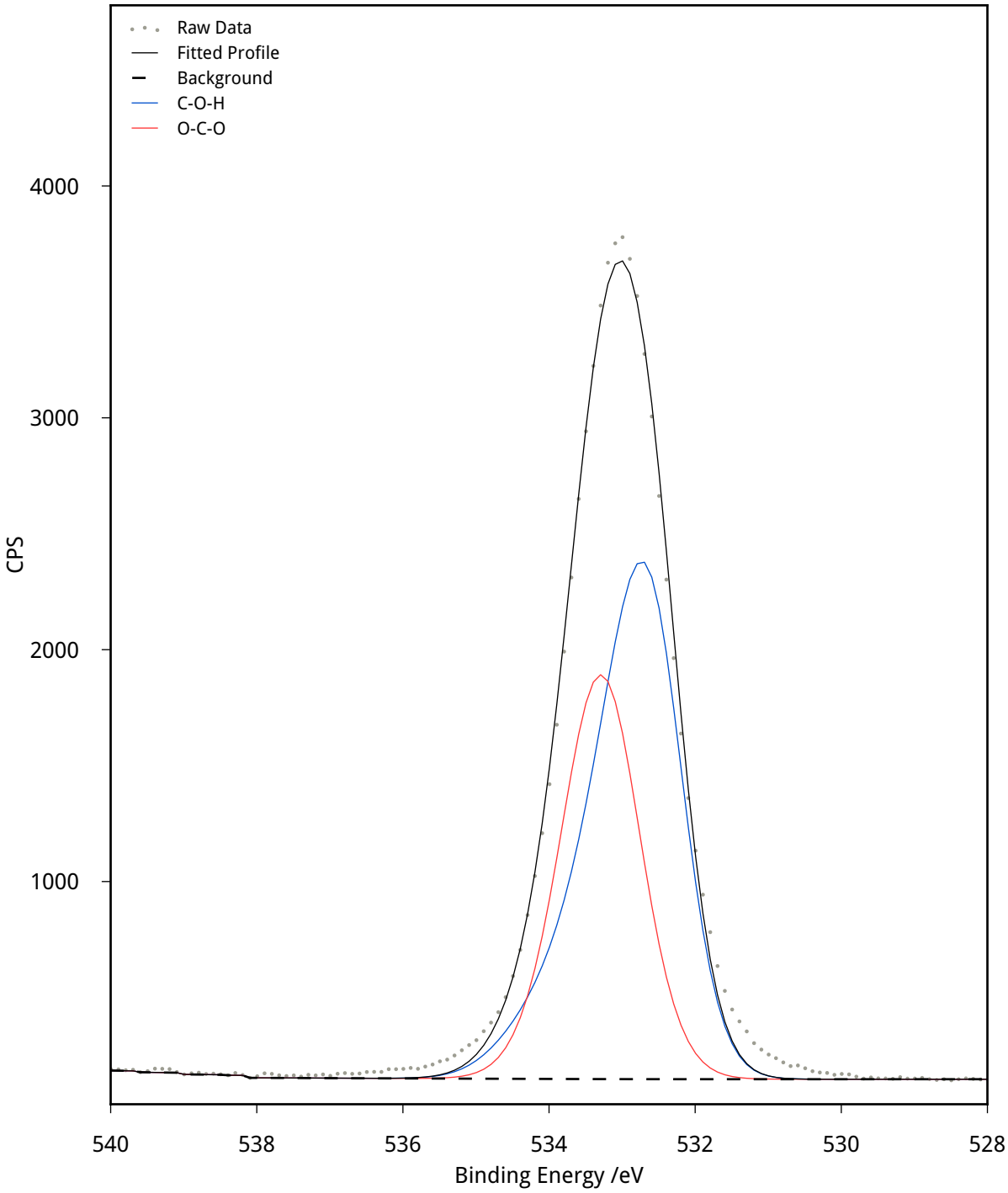

Fig. S3.6 XPS oxygen 1s high resolution scan of ImBnOO-g-CNCs

S3.5 Sulfur 2p scans

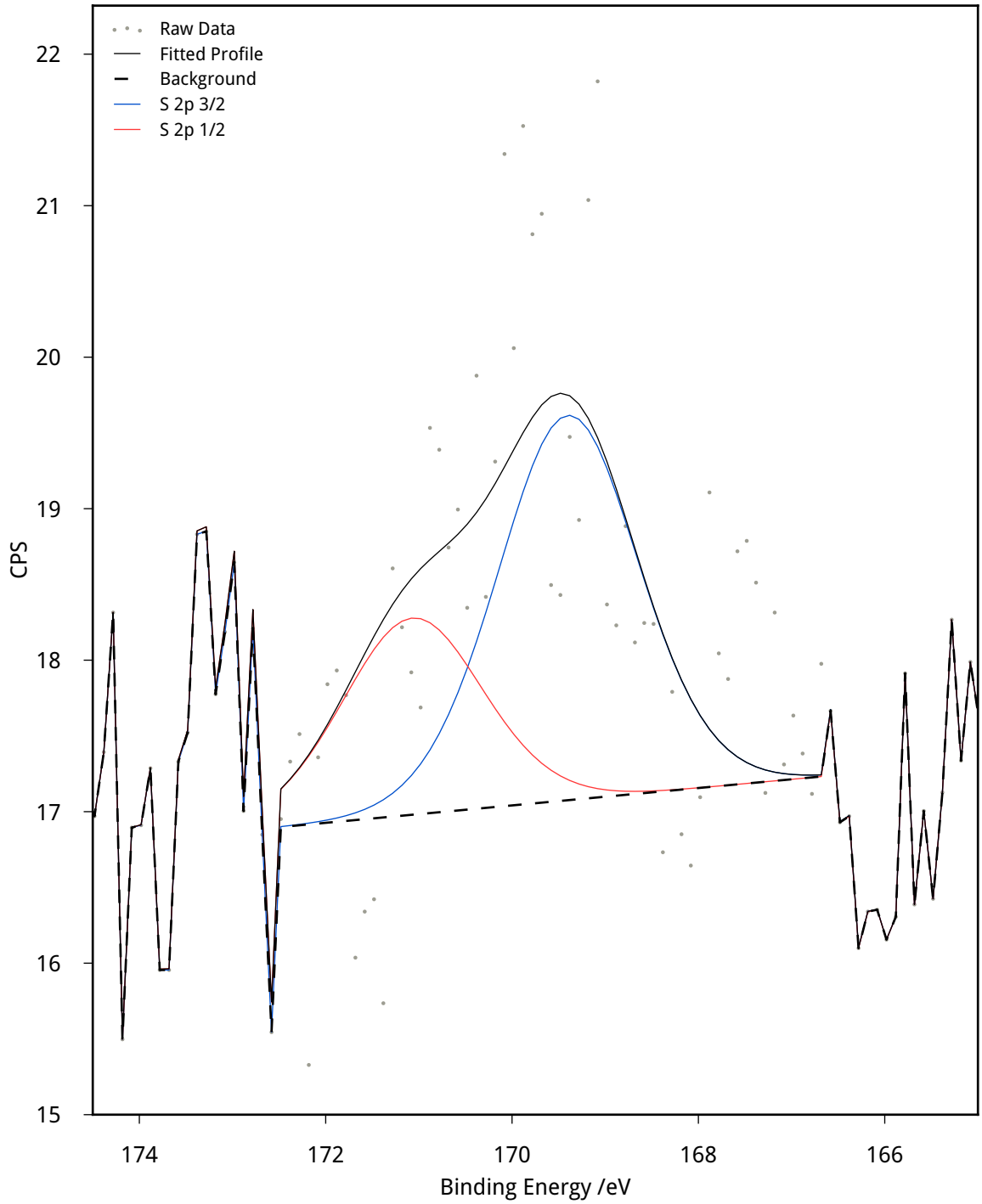

Fig. S3.7 XPS sulfur 2p high resolution scan of CNCs

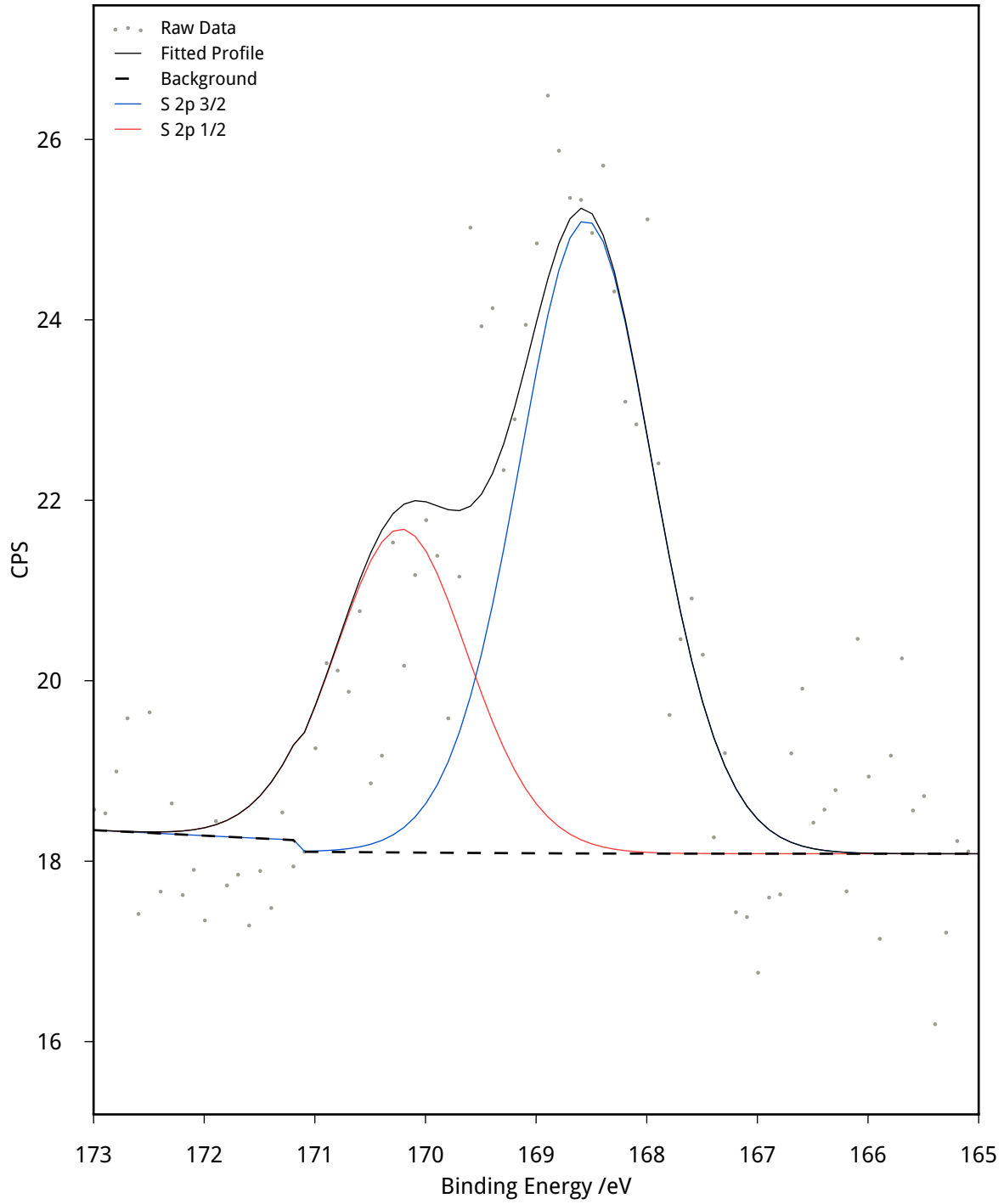

Fig. S3.8 XPS sulfur 2p high resolution scan of ImBnOO-g-CNCs

S3.6 Nitrogen 1s scans

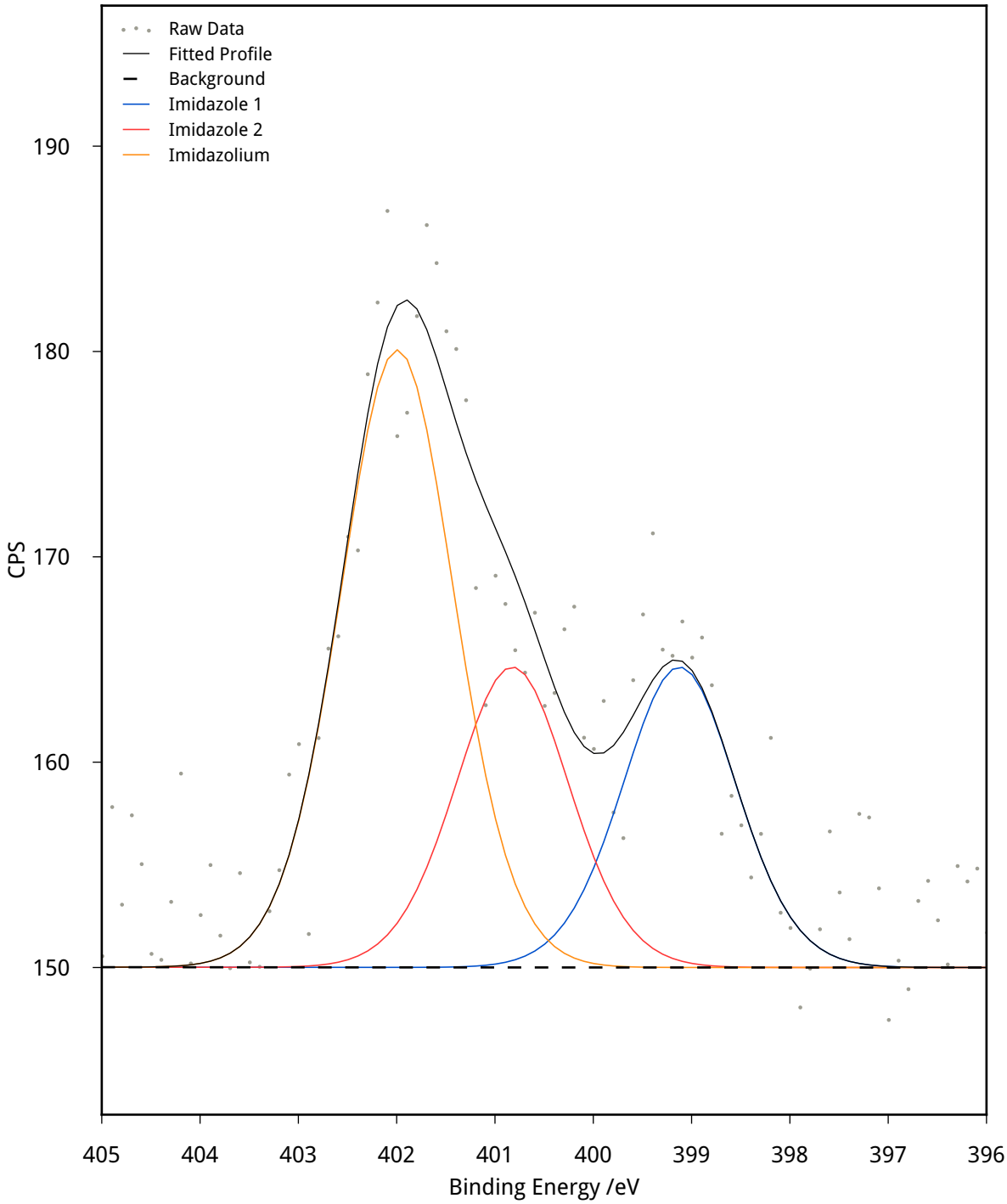

Fig. S3.9 XPS nitrogen 1s high resolution scan of ImBnOO-g-CNCs

S3.7 Chlorine 2p scans

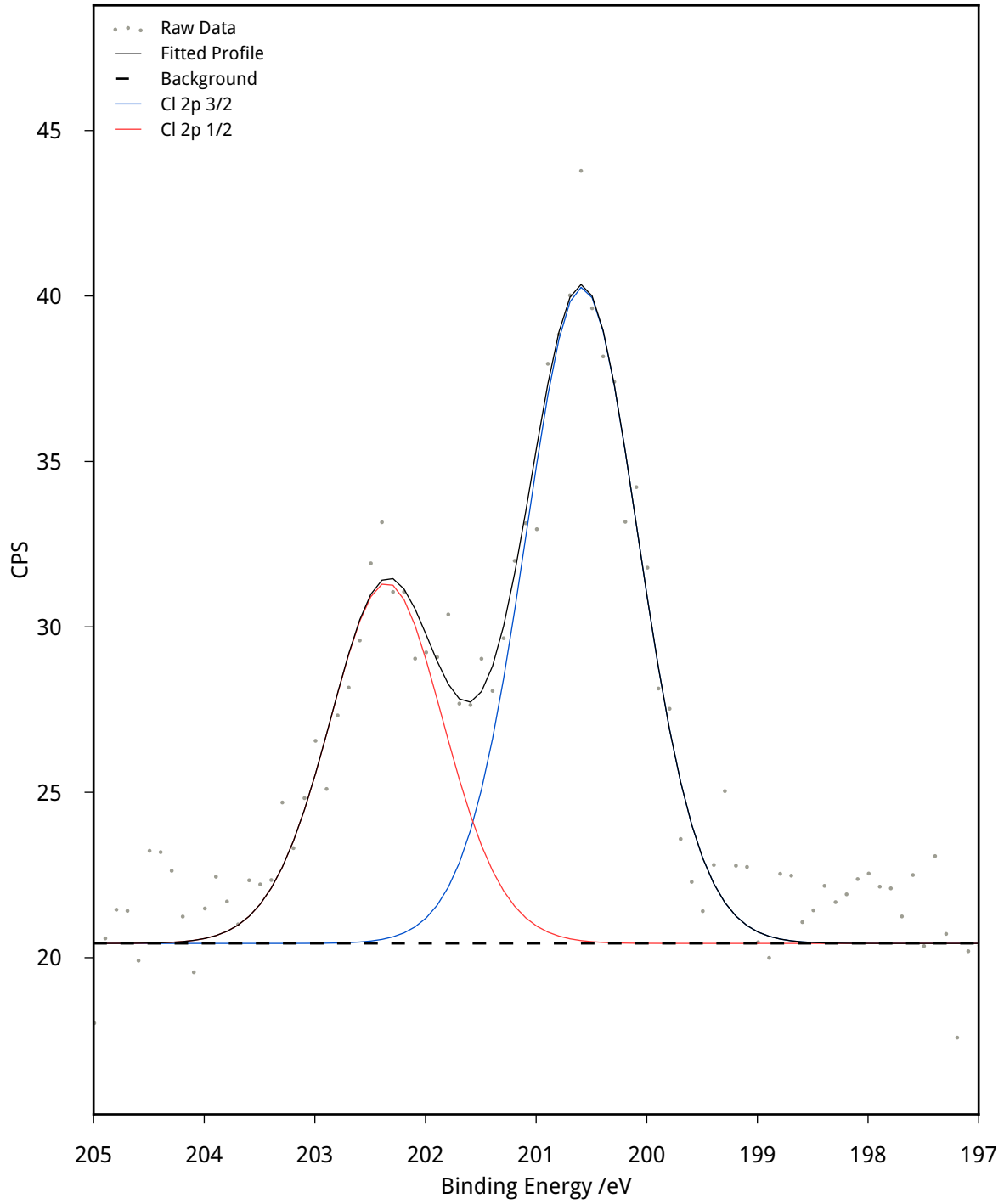

Fig. S3.10 XPS chlorine 2p high resolution scan of ImBnOO-g-CNCs

S3.8 Bromide 3d scans

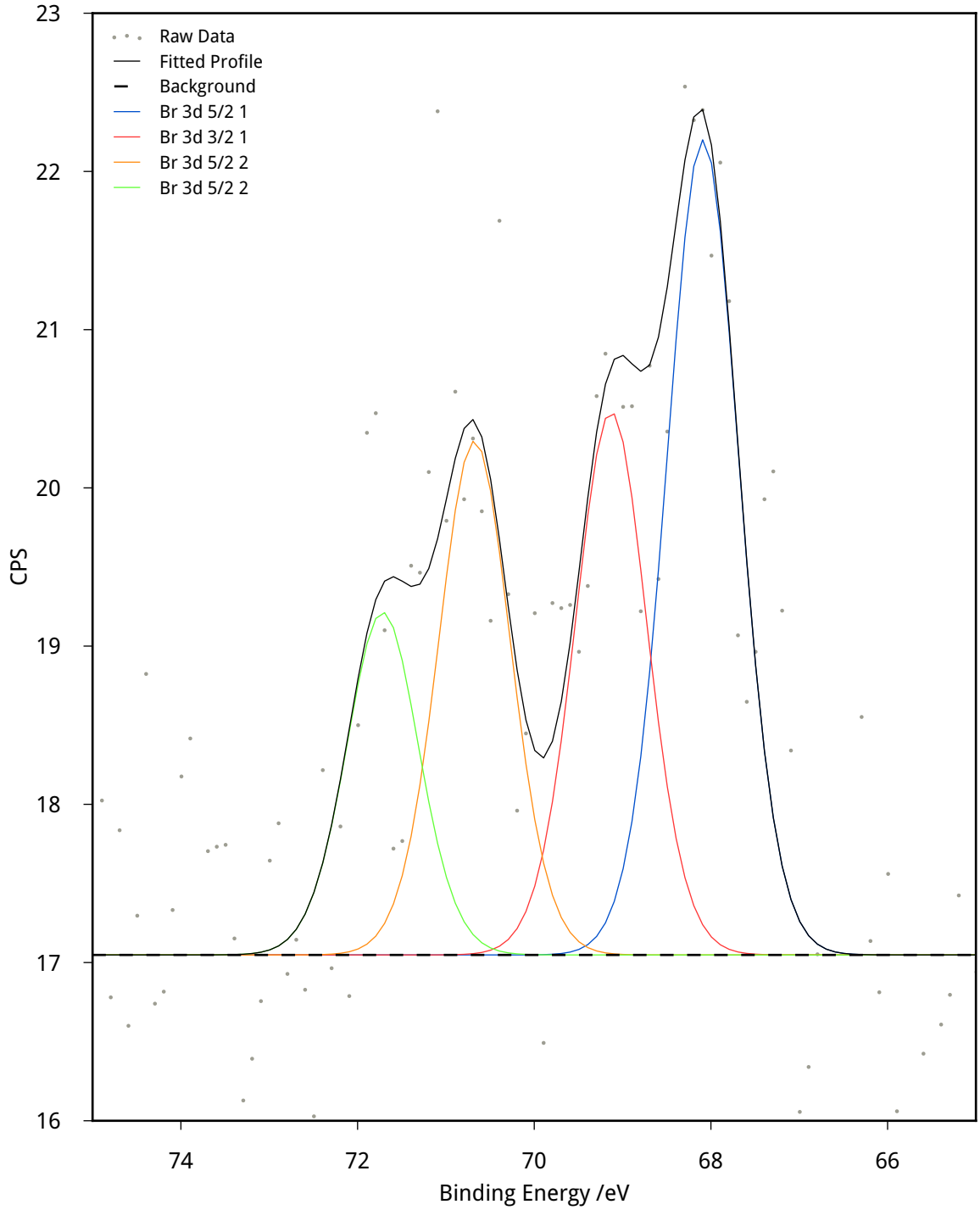

Fig. S3.11 XPS bromine 3d high resolution scan of ImBnOO-g-CNCs

S4 XRD

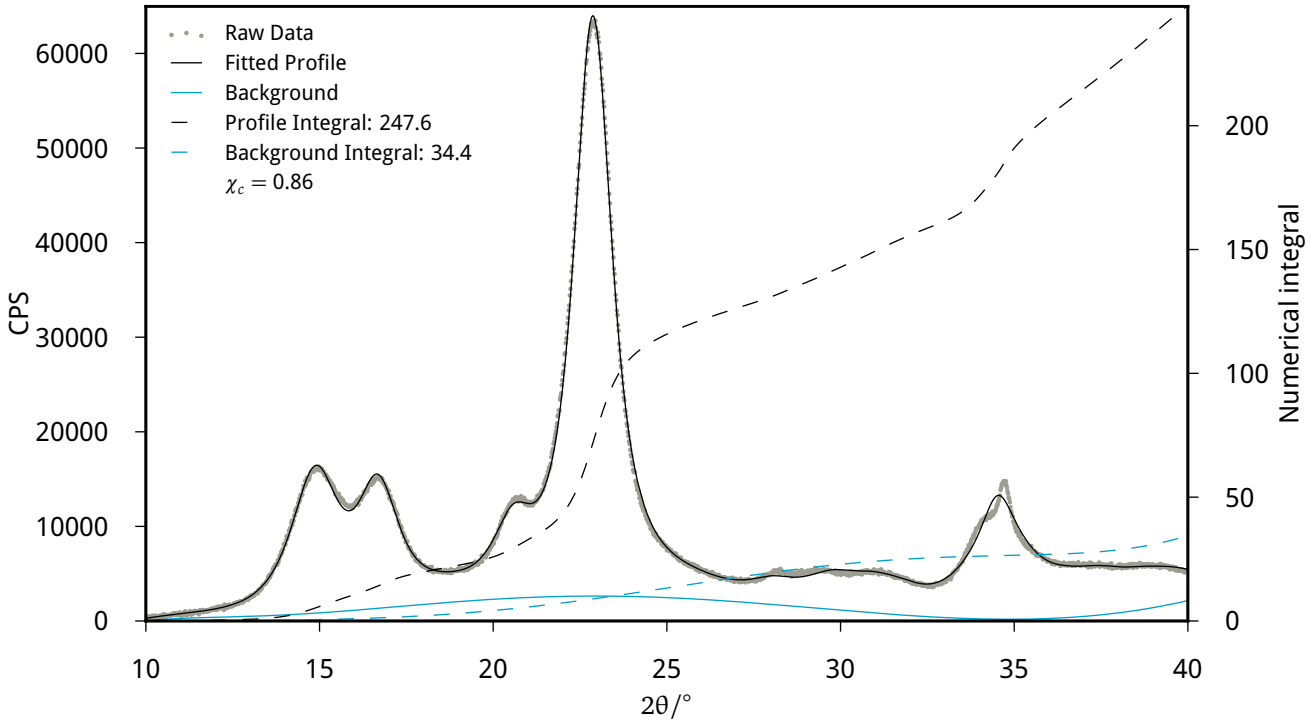

Fig. S4.1 X-ray diffractogram of CNCs showing integral curves, and calculated crystallinity index.

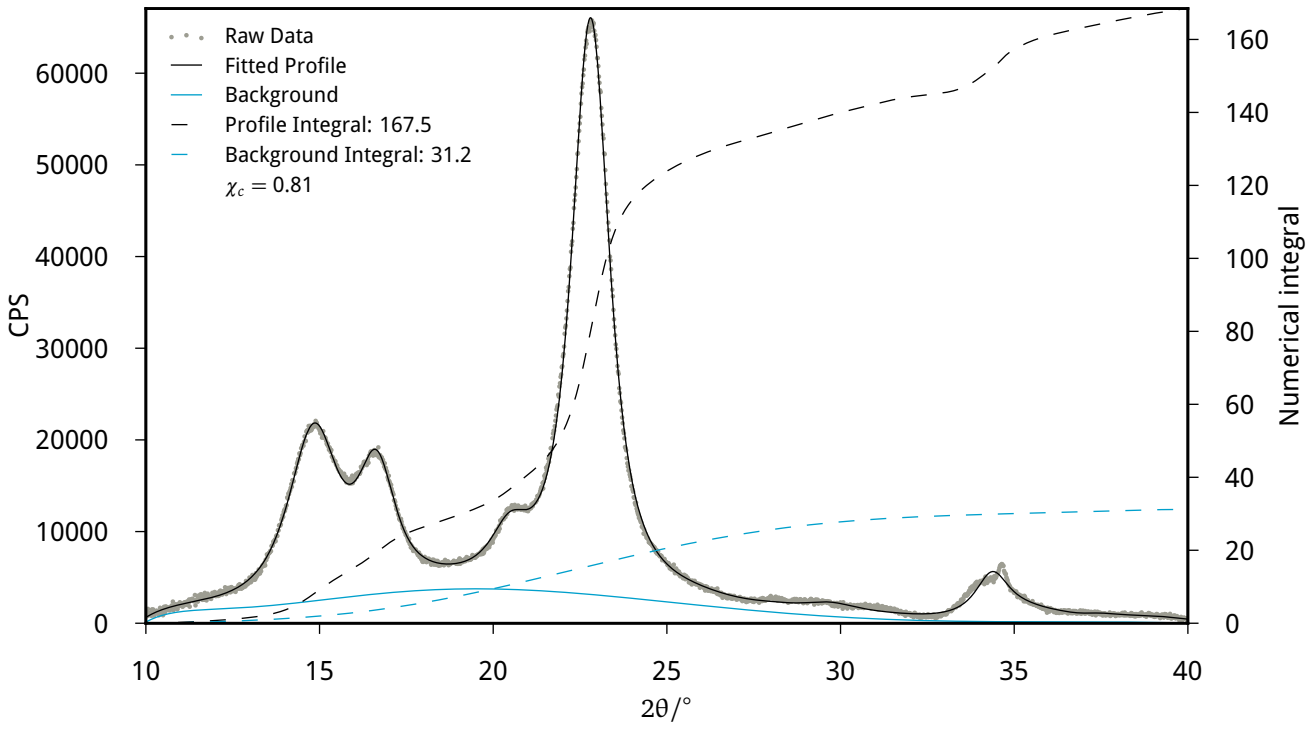

Fig. S4.2 X-ray diffractogram of ImBnOO-g-CNCs showing integral curves, and calculated crystallinity index.

Bibliography

[1] *Thermo Scientific XPS Knowledge Base - Sulfur*, accessed April 2015, http://xpssimplified.com/elements/sulfur.php.

[2] D. Nolting, N. Ottosson, M. Faubel, I. V. Hertel and B. Winter, *J. A*, 2008, **130**, 8150–8151.

[3] *Thermo Scientific XPS Knowledge Base - Bromine*, accessed April 2015, http://xpssimplified.com/elements/bromine.php.