

Covalently bonded surface functional groups on carbon nanotubes: from molecular modelling to practical applications

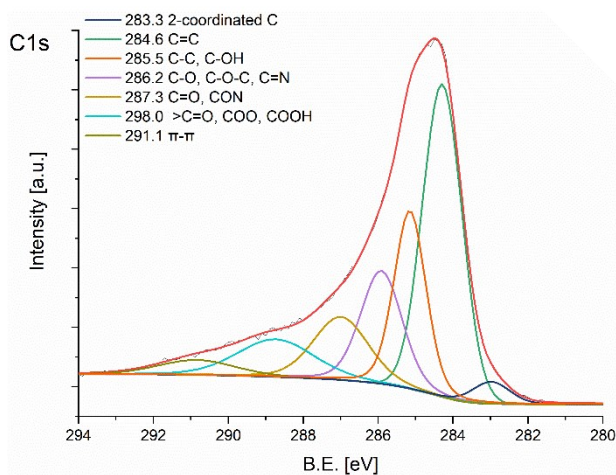
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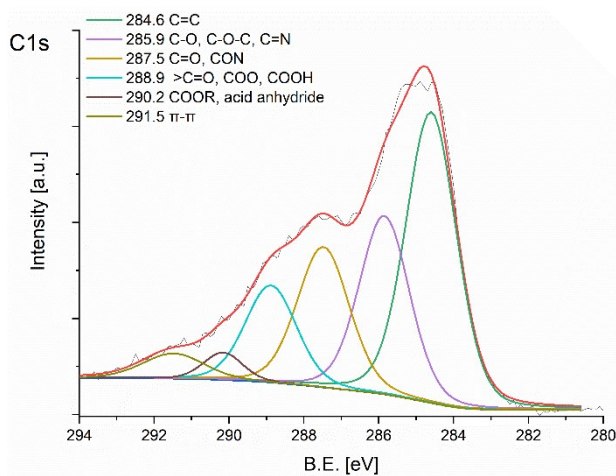
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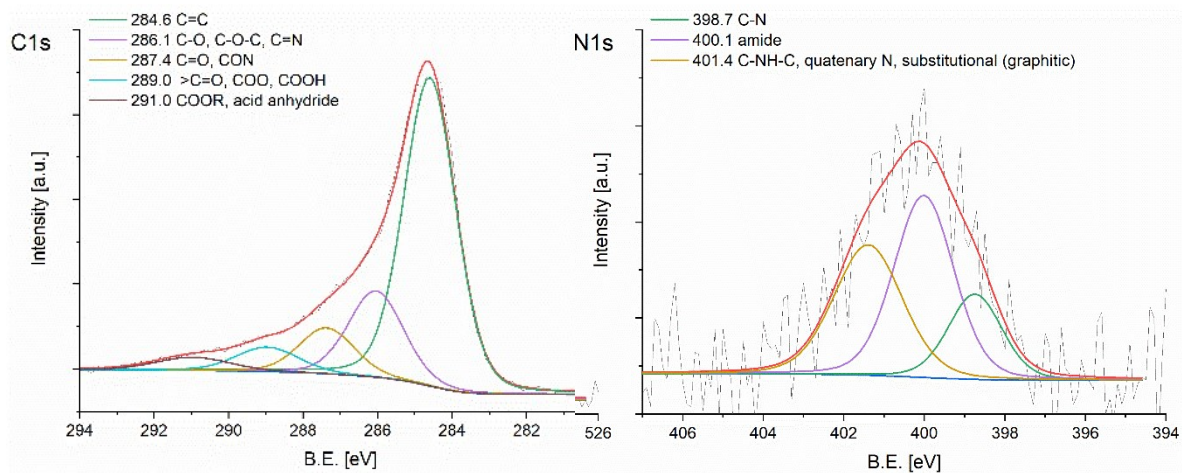
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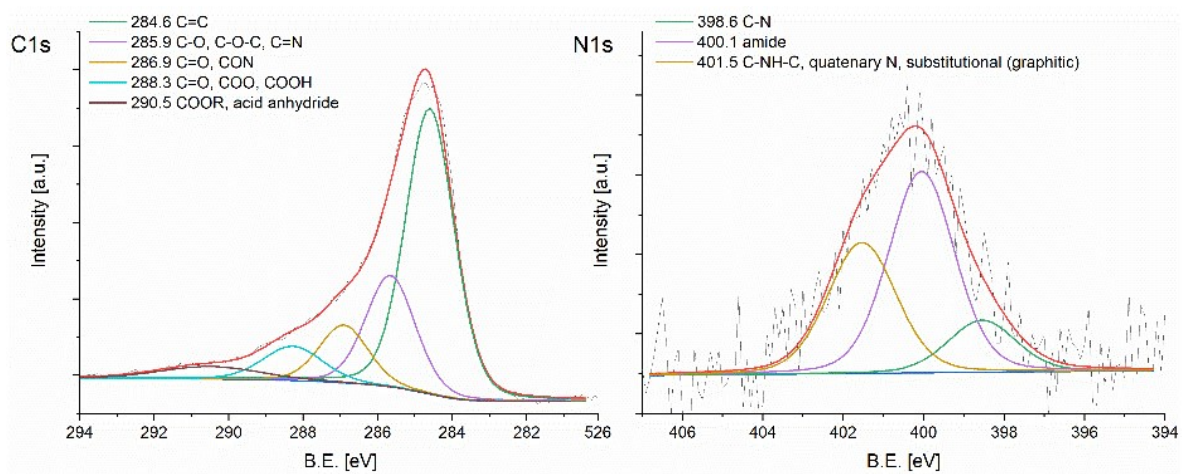
SM 1 Results of the XPS peak deconvolution of the carbon atoms present in the LO sample.



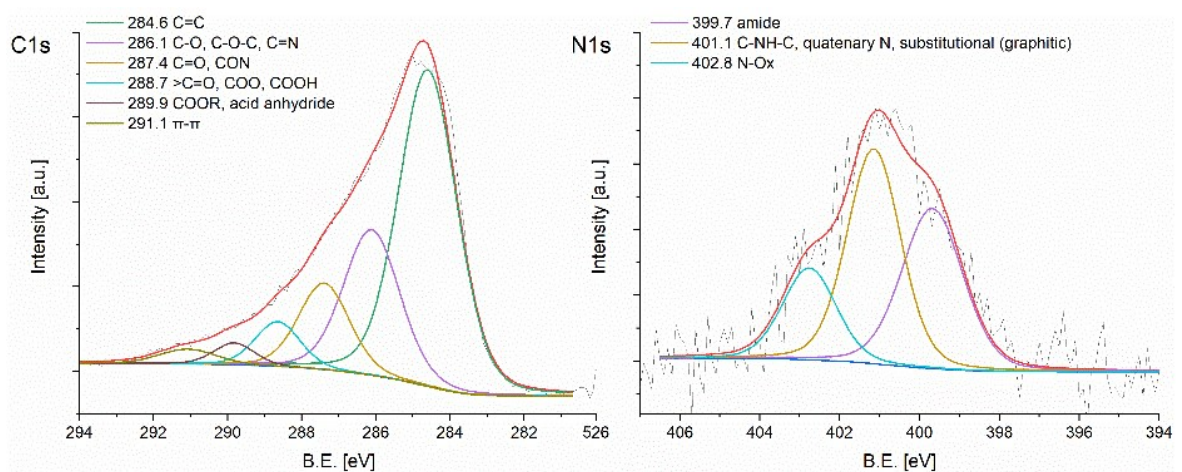
SM 2 Results of the XPS peak deconvolution of the carbon atoms present in the HO sample.



SM 3 Results of the XPS peak deconvolution of the carbon and nitrogen atoms present in the LNH sample.



SM 4 Results of the XPS peak deconvolution of the carbon and nitrogen atoms present in the HNH sample.



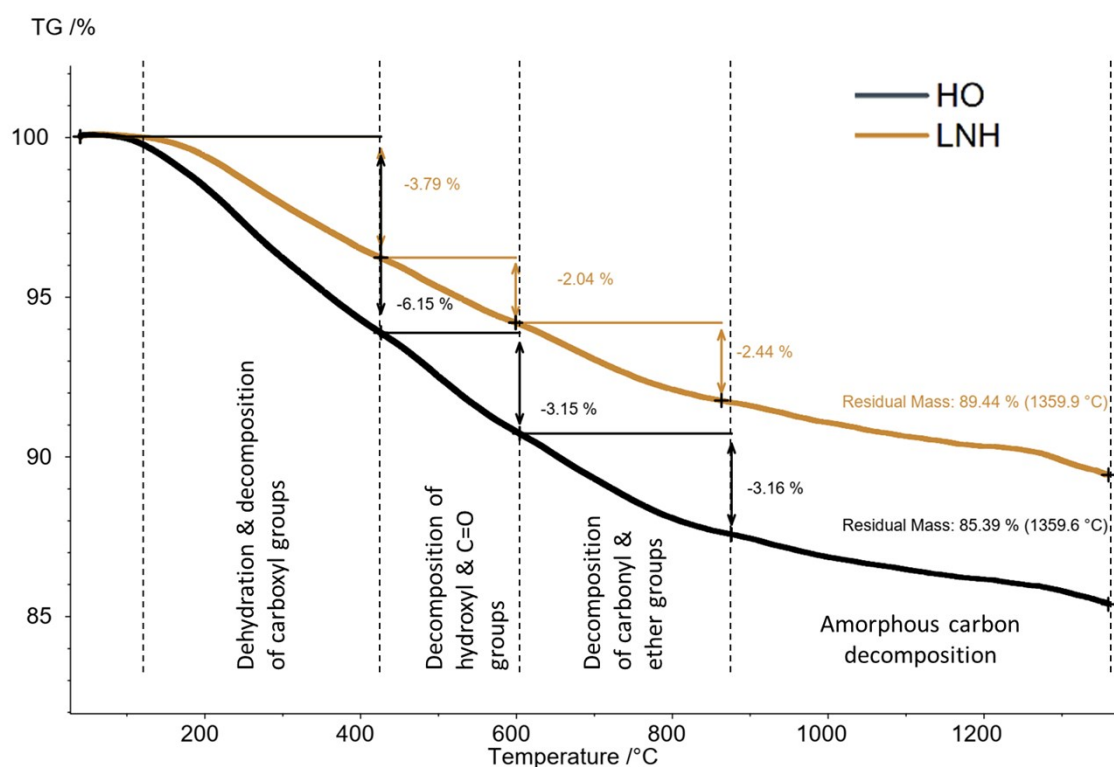
SM 5 Results of the XPS peak deconvolution of the carbon and nitrogen atoms present in the HDEA sample.

SM Table 1 XPS data for the C1s envelope of the investigated materials

B.E [ev]	Carbon species	LO	HO	LNH	HNH	HDEA
		at.%	at.%	at.%	at.%	at.%
283.3	2-coordinated C	2.3	-	-	-	-
284.6	C=C	31.9	32.1	53.5	46.7	44.4
285.5	C-C, C-OH, C-N	16.2	-	-	-	-
285.9-286.2	C-O, C-O-C, C=N	13.3	19.5	15.8	18.4	19.7
286.9-287.5	C=O, CON	9.9	15.9	8.4	9.5	10.5
288.3-289.0	>C=O, COO, COOH	8.2	10.8	5.1	6.8	4.8
290.0-290.9	COOR, acid anh.	-	2.3	3.2	4.2	4.2
291.1-291.3	π - π	3.3	3.4	-	-	2.0

SM Table 2 XPS data for the N1s envelope of the investigated materials.

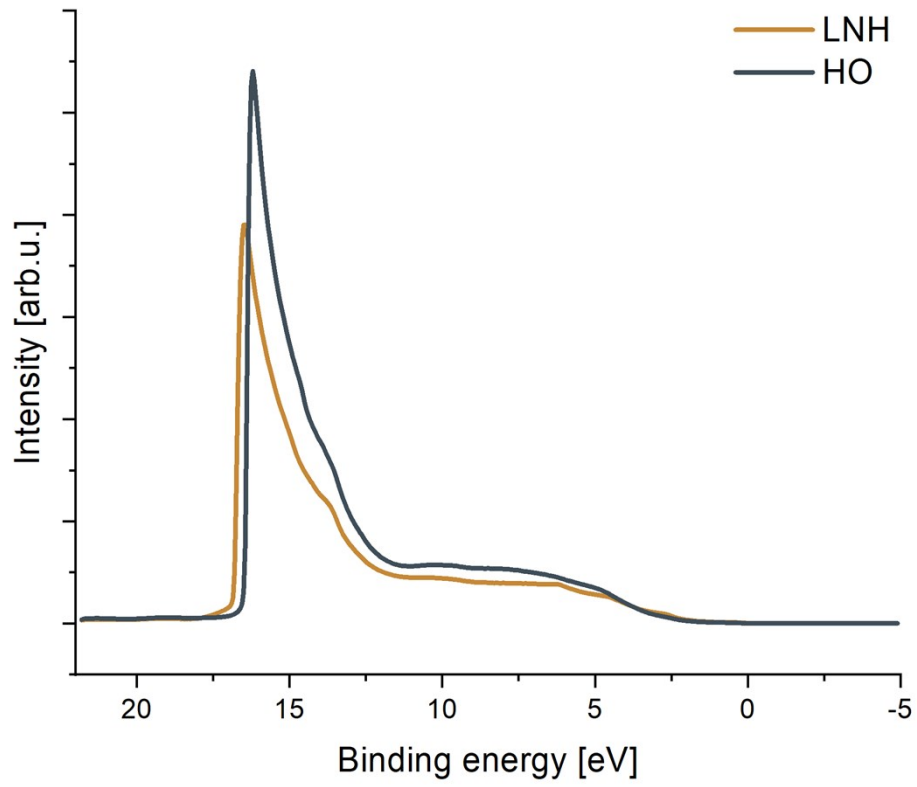
B.E [ev]	Nitrogen species	LNH	HNH	HDEA
		at.%	at.%	at.%
398.5-398.7	C-N	0.4	0.3	
400.1	amide	0.9	1.2	0.8
401.5	C-NH-C, quaternary N, substitutional (graphitic)	0.7	0.8	1.0
402.8	N-Ox			0.4



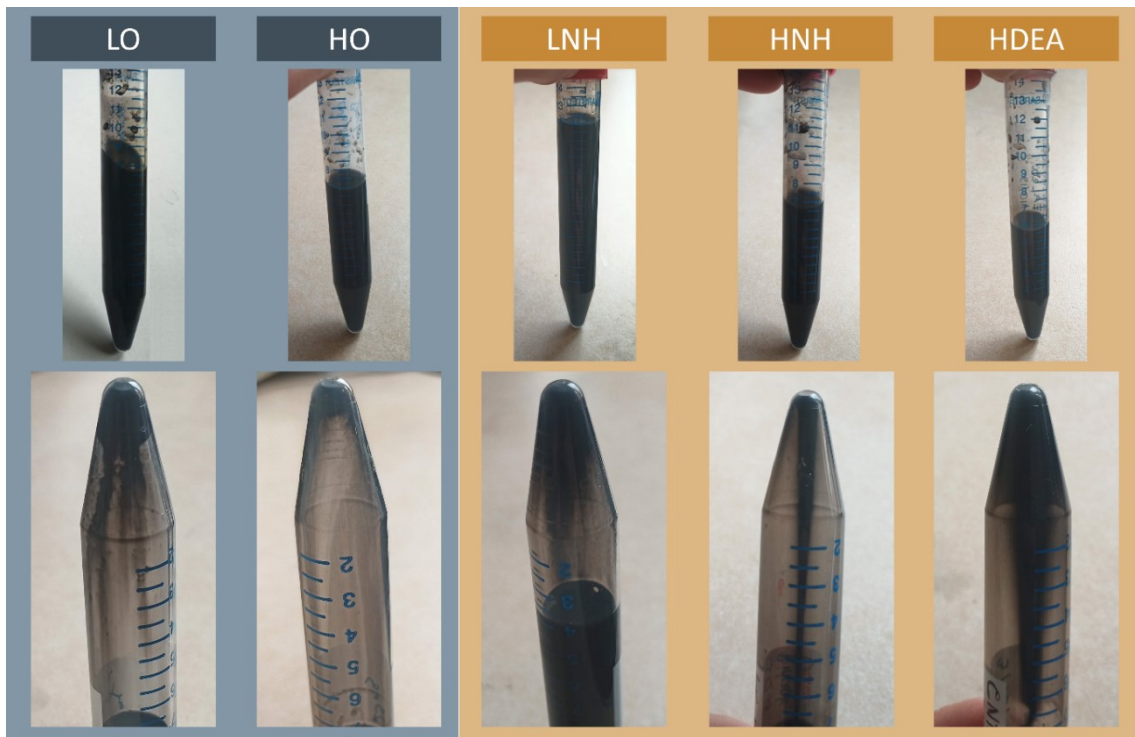
SM 6 TG curves obtained by heating the HO and LO samples up to 1360°C

SM Table 3 Raman data of the peaks' positions and areas of the investigated materials.

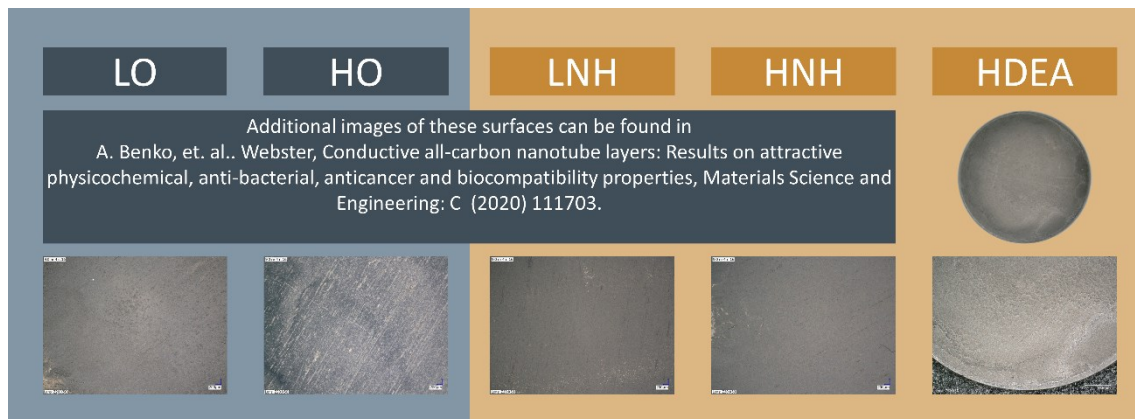
Material		position	area	FWHM	D/G	2D/G
MWCNTs	D	1346.3	41.4	46.1	1.0	1.7
	G	1572.6	40.7	36.9		
	D'	1629.9	41.9	76.8		
	2D	2688.4	68.1	78.2		
LO	D	1345.1	51.2	51.2	1.7	1.4
	G	1572.1	30.9	41.6		
	D'	1624.9	37.4	81.9		
	2D	2687.0	42.0	91.5		
HO	D	1344.0	47.2	48.5	1.7	1.6
	G	1570.5	28.0	36.1		
	D'	1628.0	40.3	76.2		
	2D	2685.9	45.2	79.8		
LNH	D	1344.7	26.4	47.8	1.2	1.7
	G	1570.4	22.4	36.0		
	D'	1633.4	34.3	76.5		
	2D	2686.4	38.4	82.3		
HNH	D	1343.0	45.6	45.8	1.4	1.6
	G	1568.5	33.0	35.3		
	D'	1627.3	46.1	75.7		
	2D	2682.2	51.3	78.3		
HDEA	D	1346.3	47.6	51.3	1.3	1.4
	G	1572.9	35.5	41.0		
	D'	1631.1	45.9	77.9		
	2D	2688.9	51.4	82.5		



SM 7 UPS spectra of the two representative samples.



SM 8 Macroscopic investigation of the CNTs dispersions, 3 months after preparation



SM 9 Images of the deposits, observed through a digital, optical microscope