

SUPPORTING INFORMATION

Acid-base properties of N-doped CNTs: A combined TPD, XPS, and 2-propanol reaction investigation

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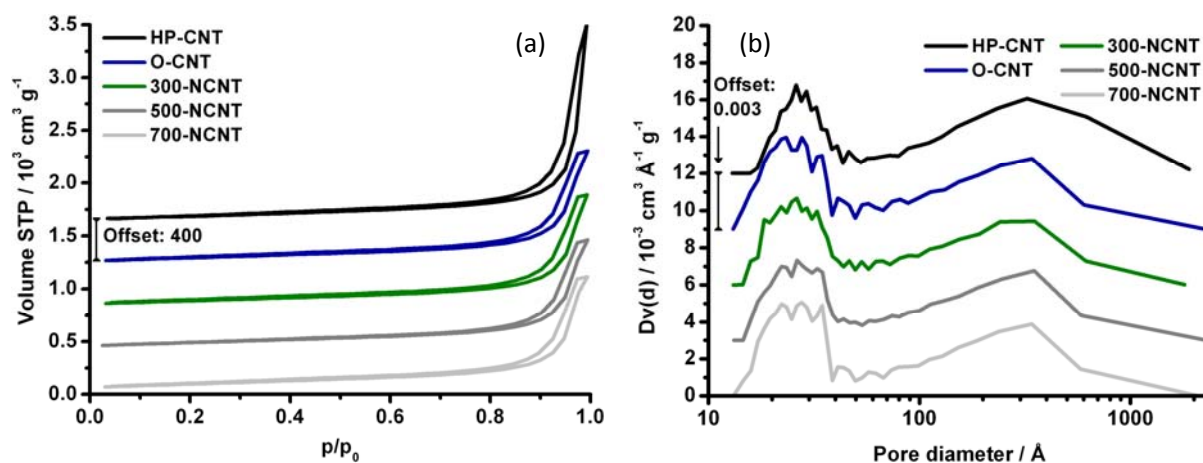


Figure S1. (a) N_2 adsorption isotherms and (b) pore size distributions of pristine and functionalized CNTs.

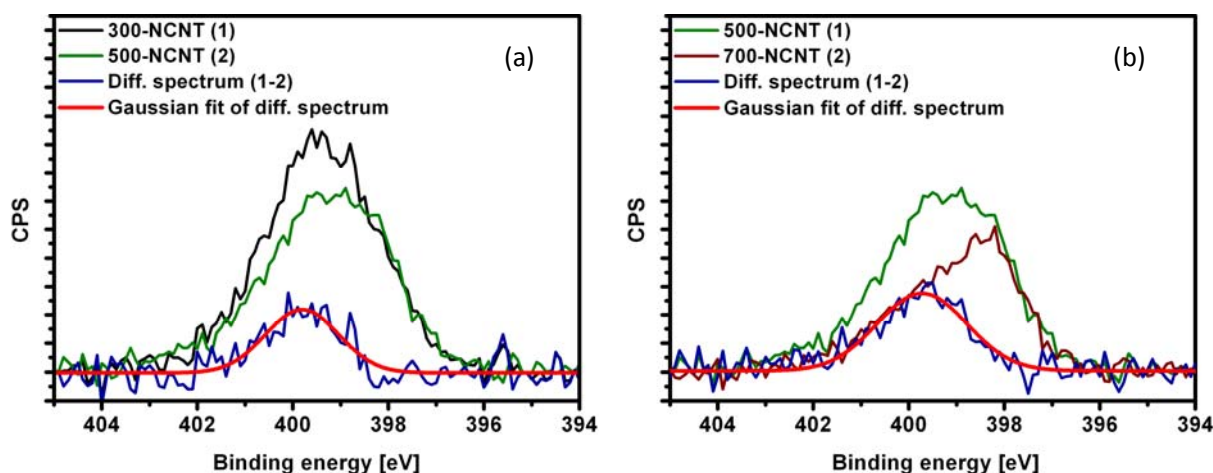


Figure S2. N_{1s} ranges of XP difference spectra of (a) 300-NCNT and 500-NCNT and (b) 500-NCNT and 700-NCNT.

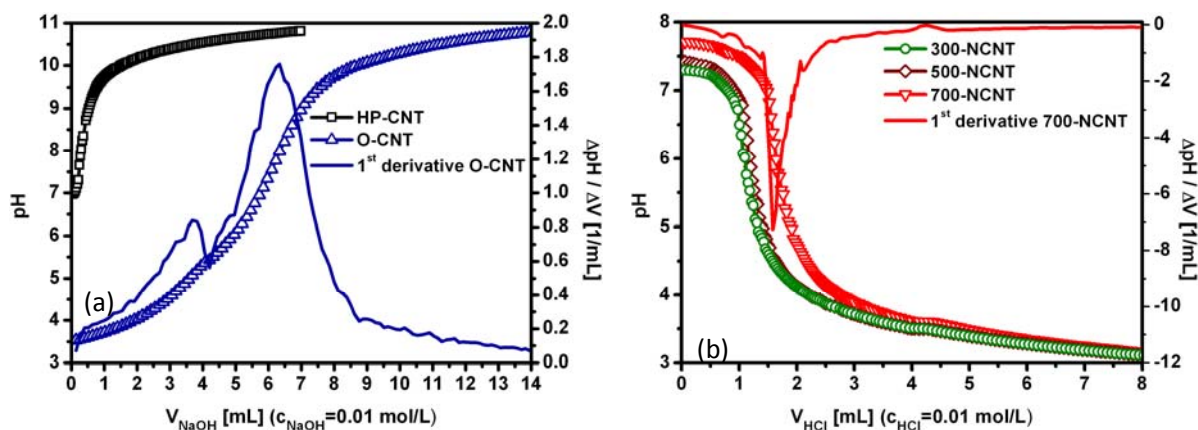


Figure S3. Potentiometric pH titration curves of (a) HP-CNT before and after HNO_3 oxidation and (b) NCNTs obtained after NH_3 treatment of O-CNT at 300, 500, and 700 °C.

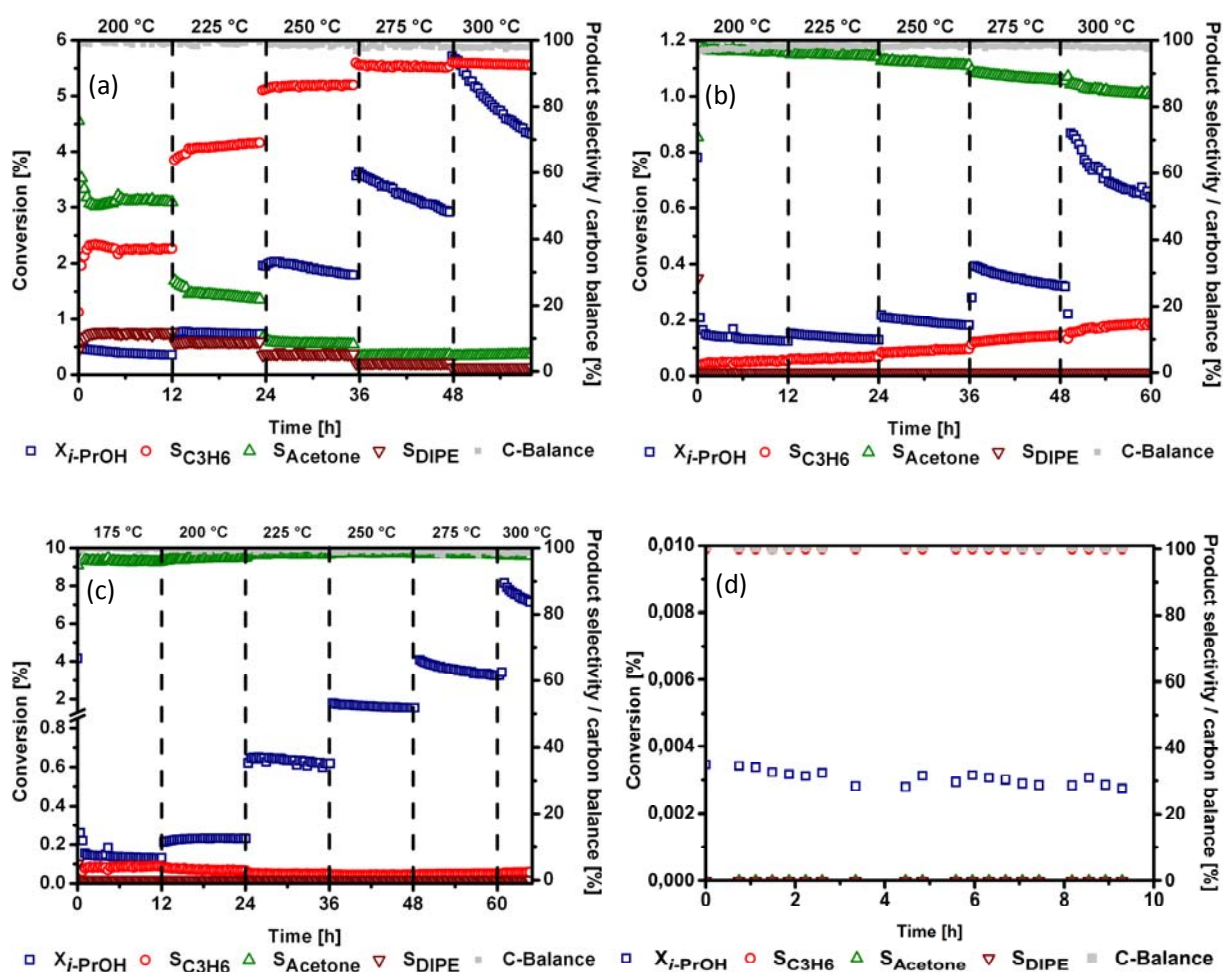


Figure S4. Conversion and selectivity as a function of time on stream obtained at five different temperatures during the catalytic decomposition of 2-propanol on (a) 300-NCNT, (b) 500-NCNT, (c) 700-NCNT, and at 200 °C on (d) HP-CNT.

Table S1. Elemental composition of NCNTs after catalytic decomposition of 2-propanol.

ID ^a	Sample	Description	Elemental analysis [wt%]			
			C	H	N	O ^b
17773	300-NCNT-ar	300-NCNT, after reaction	96.9	0.1	1.0	2.0
17772	500-NCNT-ar	500-NCNT, after reaction	96.0	0.1	1.2	2.7
17771	700-NCNT-ar	700-NCNT, after reaction	95.5	0.1	1.1	3.3

^a Internal sample number to distinguish reproductions of sample preparation

^b Oxygen is calculated as difference to 100%.

Table S2. Characteristic temperatures and heats of combustion derived from TG and DSC results.

Sample	T _{Onset} [°C]	T ₅₀ [°C]	T _{Max,DSC} [°C]	FWHM _{DSC} [°C]	ΔH _C [kJ]/g _{Sample}
HP-CNT	564	580	582	25	- 23.8
O-CNT	538	567	571	68	- 27.0
300-NCNT	542	557	557	23	- 27.6
500-NCNT	525	538	541	32	- 25.9
700-NCNT	569	582	584	26	- 26.9

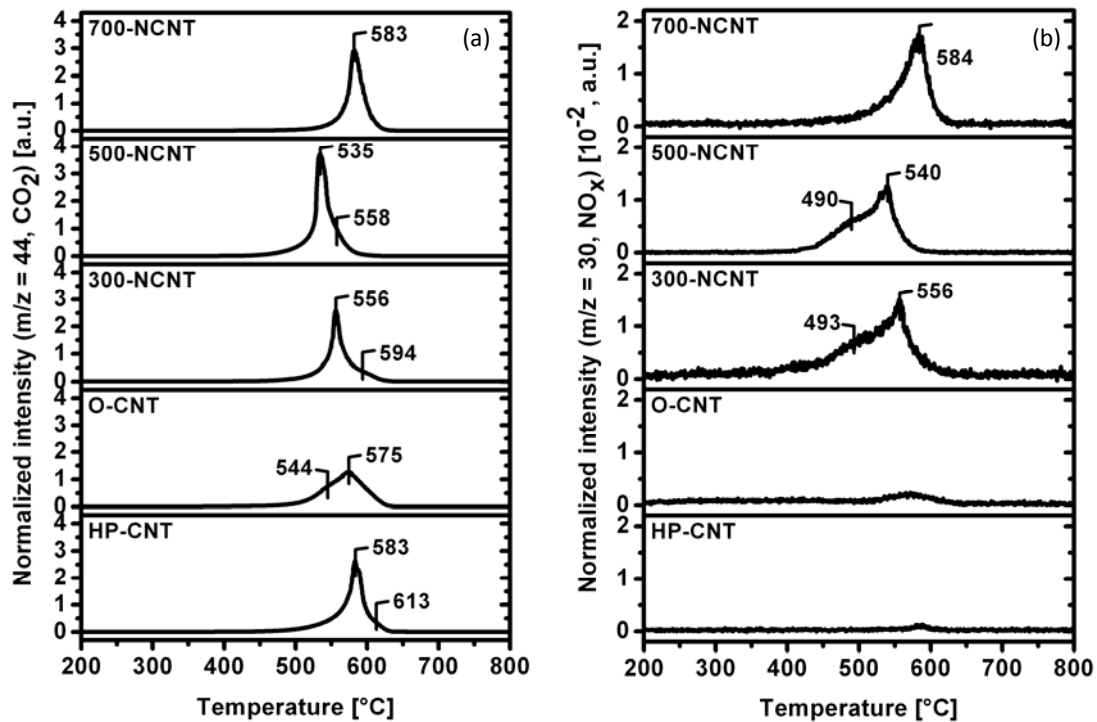


Figure S5. Mass traces recorded during TPO experiments of HP-CNT, O-CNT, and NCNTs. CO₂ [m/z = 44] (a) and NO_x [m/z = 30] (b) were normalized with respect to Ar [m/z = 40] and the employed sample mass.

Table S3. Band assignments and fitting parameters of XPS analyses (FWHM = 1.6 eV).

Species	Assignment	BE / eV	OCNT	300-NCNT	500-NCNT	700-NCNT
N1	pyridine	398.3	-	20.4%	39.3%	61.2%
N2	pyrrole	399.7	-	57.3%	44.4%	23.5%
N3	quaternary	401.0	-	22.3%	16.3%	15.2%
			300-NCNT - OCNT	500-NCNT - 300-NCNT	700-NCNT - 500 NCNT	
O1	pyridone	530.7	-	10.7%	54.1%	
O2	quinone	531.1- 531.8	30.0%	23.4%	-	
O3	ether/acid	532.0	-	-	21.5%	
O4	ether/acid	532.6	30.0%	28.3%	-	
O5	hydroxyl	533.1	-	-	24.4%	
O6	hydroxyl	533.8	32.7%	28.5%	-	
O7	ads. water	535.2	7.3%	9.1%	-	