Boehm Titration Revisited (Part II): A Comparison of Boehm Titration with other Analytical Techniques on the Quantification of Oxygen-Containing Surface Groups for a Variety of Carbon Materials

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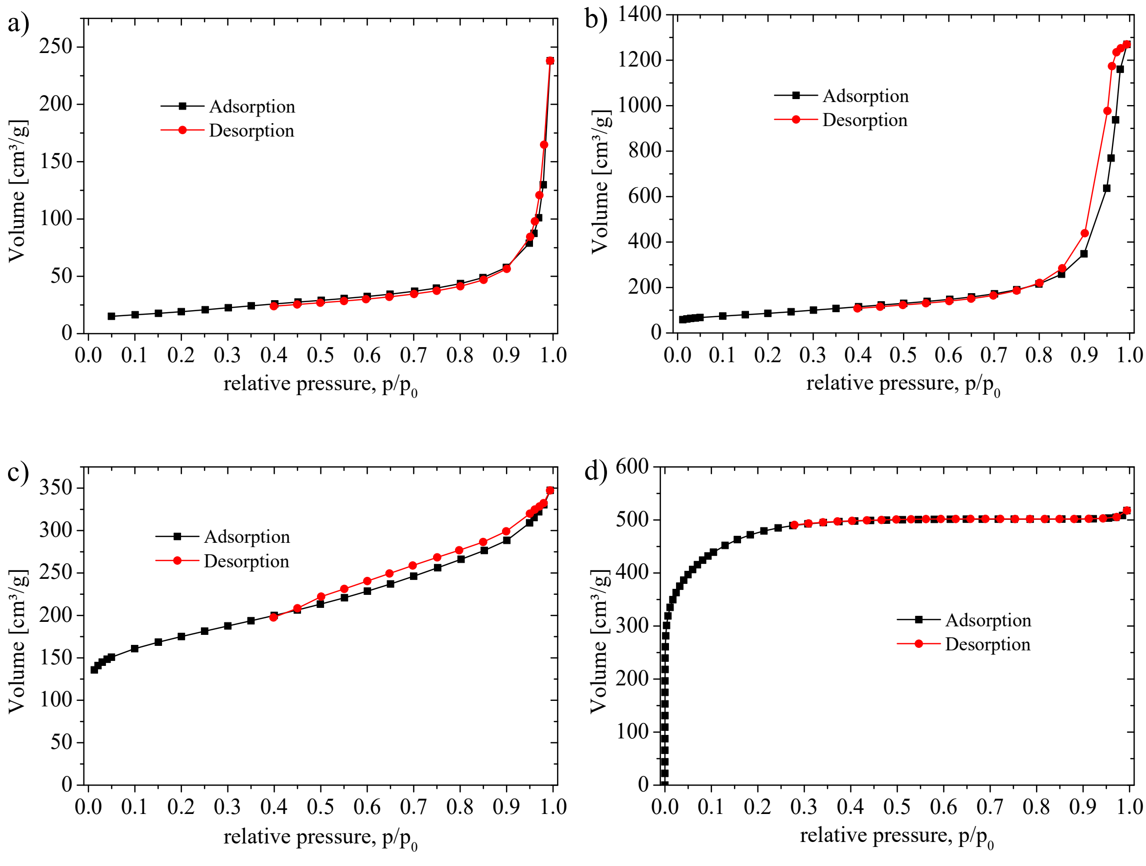

Figure S1. N_2 Isotherms of (**a**) aCB; (**b**) aCNTs; (**c**) aAC1 and (**d**) aAC2

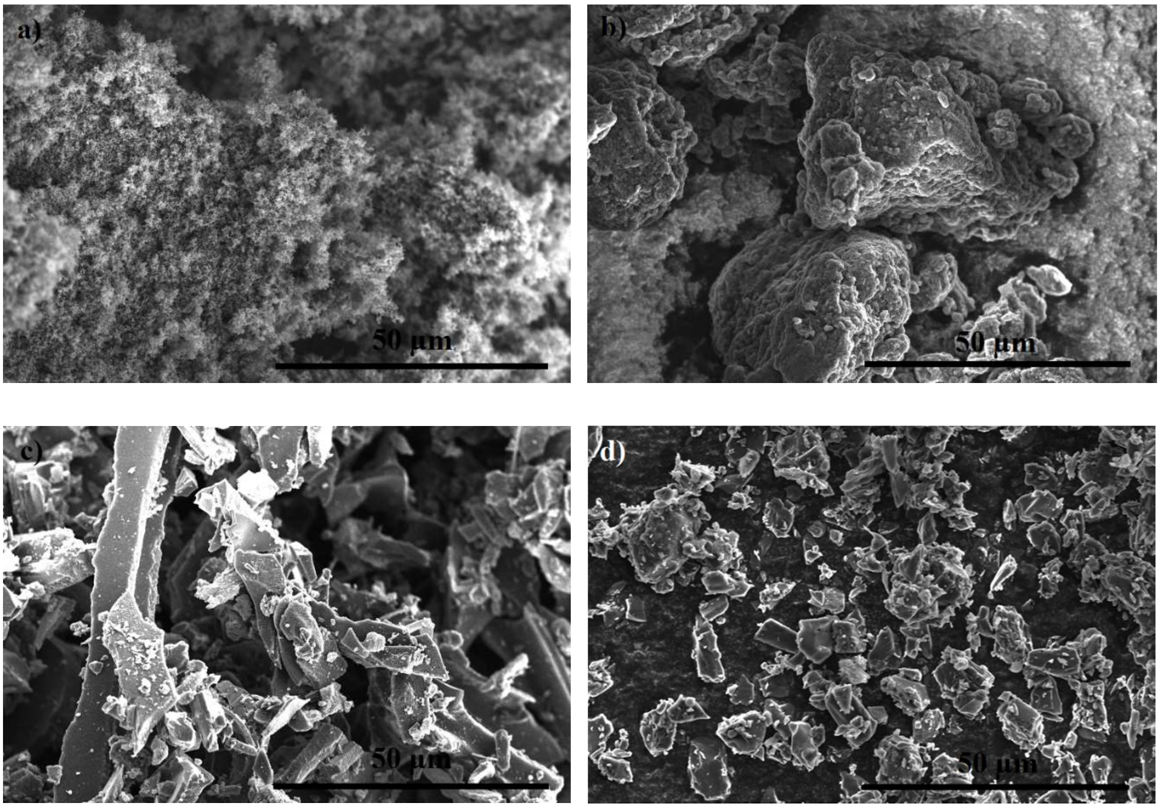

Figure S2. SEM-Images from (**a**) aCB; (**b**) aCNTs; (**c**) aAC1 and (**d**) aAC2

Table S1. Specific surface area, pore volume and micropore area of the carbon materials (*QSDFT with cylindrical pores at pore width over 2 nm).

	aCB	**aCNTs**	**aAC1**	**aAC2**
SSA [m^2/g] (BET)	68.9	307	638	1759
SSA [m^2/g] (QSDFT)	61.6	293*	650	1551
Total pore volume (at p/p_0)	0.368 (0.99406)	1.964 (0.99426)	0.5373 (0.99417)	0.8008 (0.99460)
Total pore volume (QSDFT) [cm^3/g]	0.114	1.808*	0.478	0.721
Micropore SA [m^2/g] (t-plot)	0	0	363	1553
Micropore SA [m^2/g] (QSDFT)	33.8	16.4*	520	1542

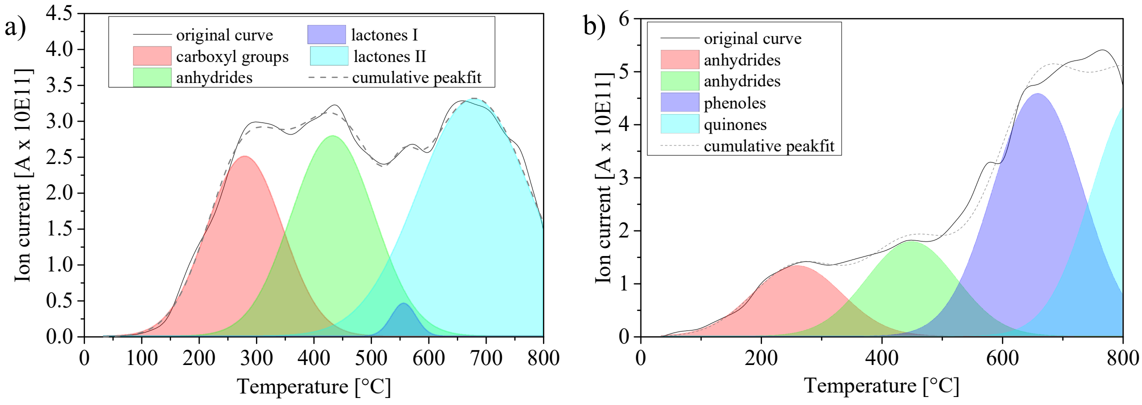

Figure S3. TPD deconvolution of (**a**) CO_2 and (**b**) CO for aAC1

Calculation of total oxygen amount for the BT (aAC2) $\left[\frac{g_{oxygen}}{g_{carbon\ material}}\right]$:

$$wt\,\%\,O = \left((\text{mass oxygen in all –COOH}) + (\text{mass oxygen in all –COO–}) + (\text{mass oxygen in all –OH})\right) \times 100\%$$

$$wt\,\%\,O = \left(\left(\frac{n_{-COOH}}{g_{carbon}} \times M_{-COOH} \times \frac{M_{2O}}{M_{-COOH}}\right) + \left(\frac{n_{-COO-}}{g_{carbon}} \times M_{-COO-} \times \frac{M_{2O}}{M_{-COO-}}\right) + \left(\frac{n_{-OH}}{g_{carbon}} \times M_{-OH} \times \frac{M_{O}}{M_{-OH}}\right)\right) \times 100\%$$

$$\left(\frac{M_{2O}}{M_{-COOH}}\right) = \text{amount of oxygen within the group}$$

$$wt\,\%\,O = \left(\left(1.02\frac{mmol}{g_{carbon}} \times 32\frac{g_O}{mol}\right) + \left(0.24\frac{mmol}{g_{carbon}} \times 32\frac{g_O}{mol}\right) + \left(0.53\frac{mmol}{g_{carbon}} \times 16\frac{g_O}{mol}\right)\right) \times 100\%$$

$$wt\,\%\,O = \left(\frac{(32.7) + (7.55) + (8.47)}{1000}\right) \times 100\%$$

$$wt\,\%\,O = 4.87\%$$

Calculation of total oxygen amount for the TPD (aAC1) $\left[\frac{g_{oxygen}}{g_{carbon\ material}}\right]$:

Assumption: $\text{mass loss}_{TGA} = m_{CO} + m_{CO2}$

$$wt\,\%\,O = \left(m_{CO} \times \frac{M_O}{M_{CO}} + m_{CO2} \times \frac{M_{2O}}{M_{CO2}}\right) \times \text{mass loss}_{TGA}\ [\%]$$

$$\text{wt \% O} = \frac{\left(A_{COOH,\ COOR}\,[\%] \times \frac{M_{2O}}{M_{CO2}} + A_{anhydride}\,[\%] \times \frac{M_{3O}}{M_{CO2+CO}} + A_{phenol}\,[\%] \times \frac{M_{O}}{M_{CO}}\right)}{100\%} \times \text{mass loss}_{TGA}\,[\%]$$

$\left(\frac{M_{3O}}{M_{CO}}\right)$ = amount of oxygen within released gas for one anhydride

$A_{COOH,\ COOR}\,[\%] = \frac{A_{COOH,\ COOR}}{\sum A_{all\ groups}}$ (A= peak area from deconvolution)

$$\text{wt \% O (aAC1)} = \frac{(32.97\% \times 0.73 + 22.07\% \times 0.67 + 22.54\% \times 0.57)}{100\%} \times 16.44\%$$

$$\text{wt \% O (aAC1)} = 8.48\%$$

(m_{CO} from quinones etc. is not included in wt % O)