Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

to

Correlation of the Electrochemistry of Poly(acrylonitrile)-Sulfur Composite Cathodes with its Molecular Structure

*Jean Fanous, Marcus Wegner, Jens Grimminger, Malte Rolff, Marcelle B. M. Spera, Martin Tenzer and Michael R. Buchmeiser**

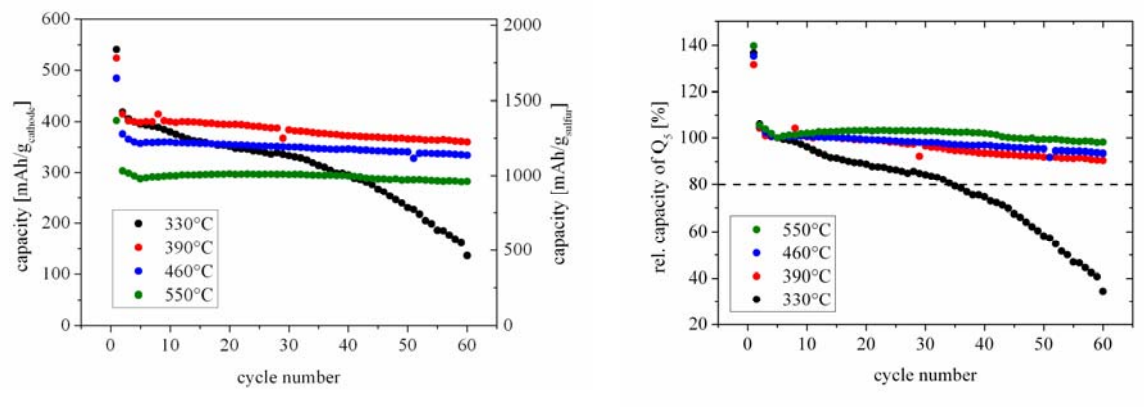

Figure S1: Influence of the synthesis temperature on cathode stability. a) absolute capacity b) relative capacity (% of Q_5).

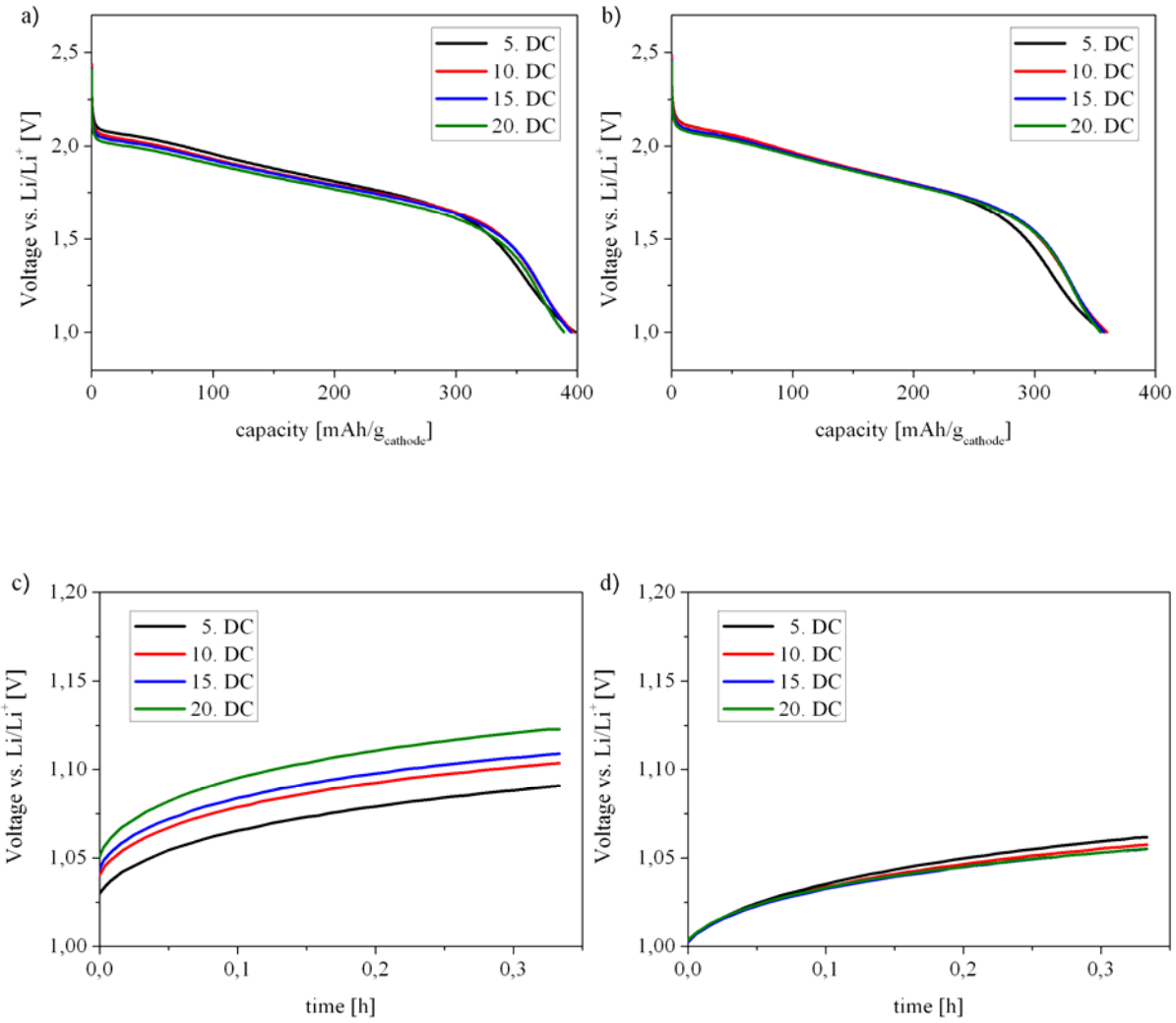

Figure S2. Voltage profile of the nth discharge (a+b) and the following pause step (c+d) of SPAN(390°C) (a+c) and SPAN(460°C) (b+d).

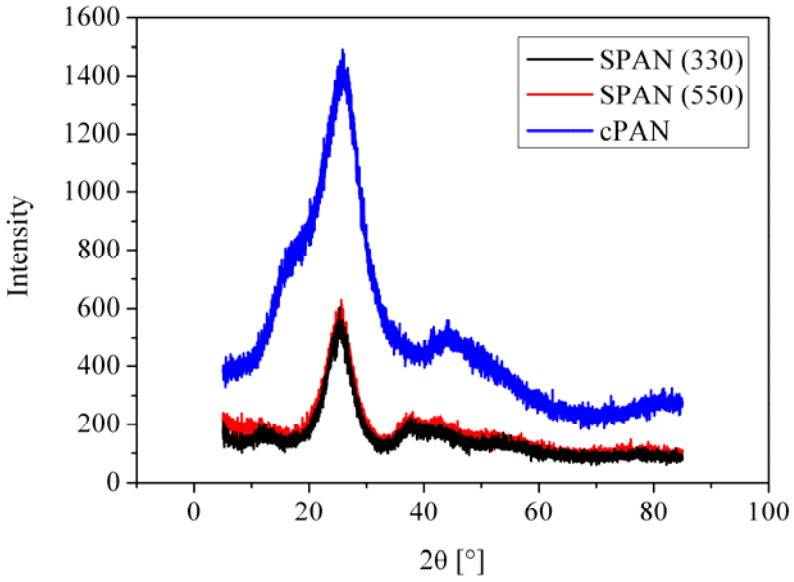

Figure S3. XRD patterns of cPAN (blue), $SPAN_{330}$ (black) and $SPAN_{550}$ (red).

Table S1. Comparison of the angular peak positions of cPAN, both SPAN samples and crystalline graphite.

Sample	**Diffraction maxima (observed) (°)**						
$SPAN_{330}$	12		25.4	37.5	42.3	53.0	
$SPAN_{550}$	12		25.4	37.5	42.6	53.1	
cPAN		17.1	25.8	36.0	44.1	51.8	81.9
graphite (data base value)			26.381				

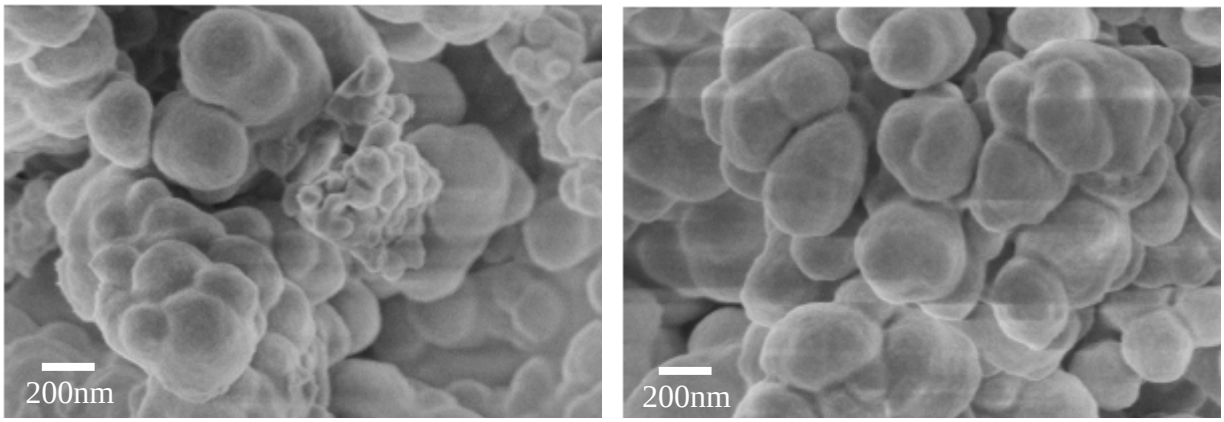

Figure S4. SEM images of $SPAN_{330}$ (left) and $SPAN_{550}$ (right).

FT-IR spectra of SPAN330 and SPAN550 are shown in Figure S4 and do not show significant differences. Only at 1545 cm-1, a very minor but sharp band is observed for SPAN330, whereas the corresponding vibration of SPAN550 appears as shoulder. However, FT-IR as a non-resonant analytical tool is – in contrast to resonance Raman spectroscopy – not sensitive enough to allow for any conclusions with regards to structural differences between both materials.

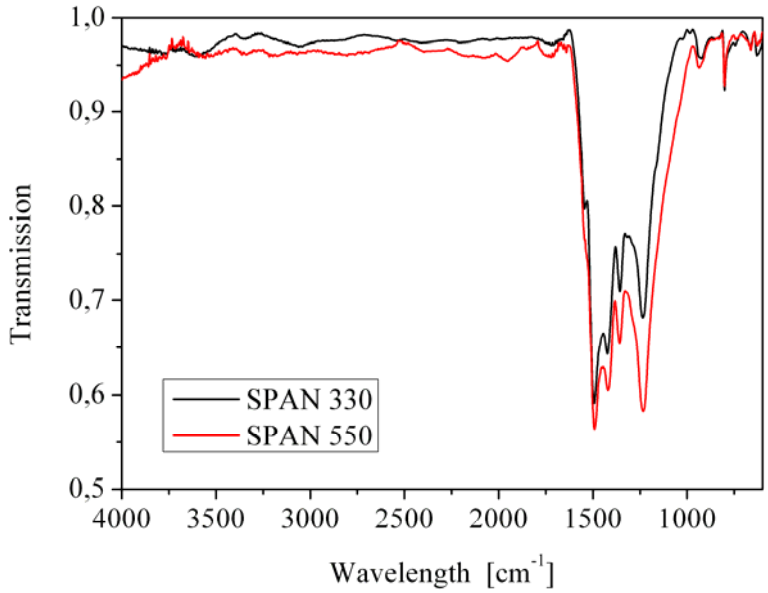

Figure S5. FTIR spectra of $SPAN_{330}$ (black) and $SPAN_{550}$ (red).

The C1s XPS spectra of cPAN, $SPAN_{330}$ and $SPAN_{550}$ are depicted in Figure S5. The ~284 eV peak was normalized to 1.0. In agreement with Yu et al., the peak at 286.5 eV is assigned to the C=N state and the peak at 284.6 eV to the C=C state.[8] The spectra of both SPAN samples do not show significant differences, suggesting similar states of the inner electrons in both materials. In contrast, cPAN reveals a different ratio of the intensities at 286 and 284 eV, as the incorporated sulphur in SPAN compensates for the electron withdrawing effect of the nitrogen by providing additional electron density within the C-S bonds. In due consequence, the intensity of the C=N state decreases with respect to the C=C state and the superimposed C-S state (285.7 eV).[8]

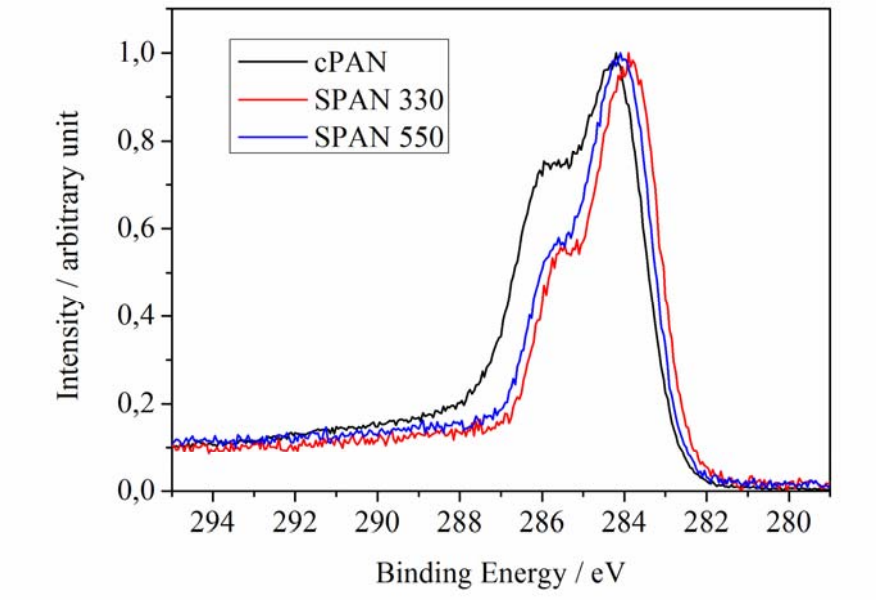

Figure S6. XPS spectra (C1s) of $SPAN_{330}$ (red), $SPAN_{550}$ (blue) and cPAN (black).

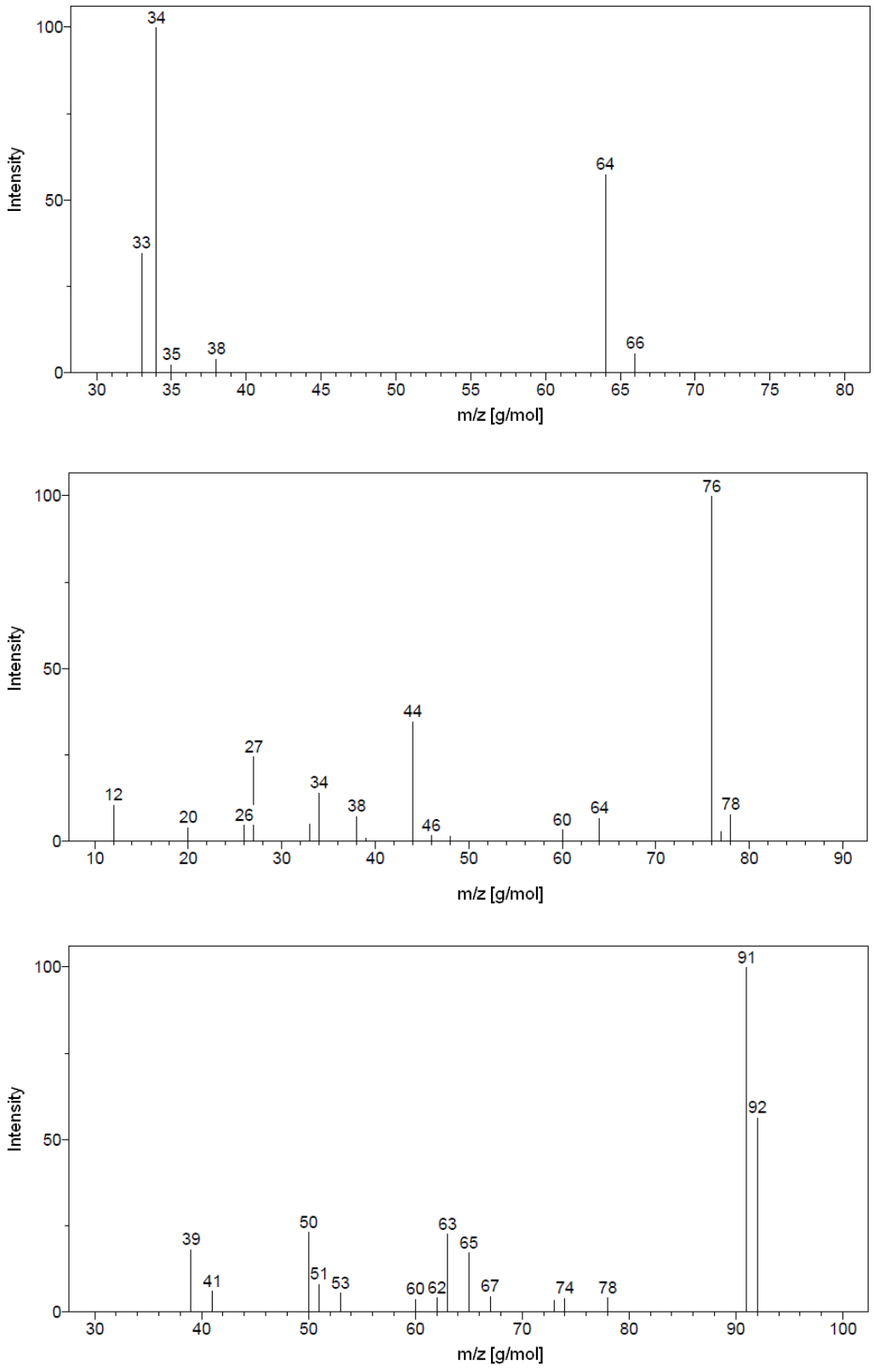

Figure S7. MS spectra of TG-MS measurements at intensity maximum.

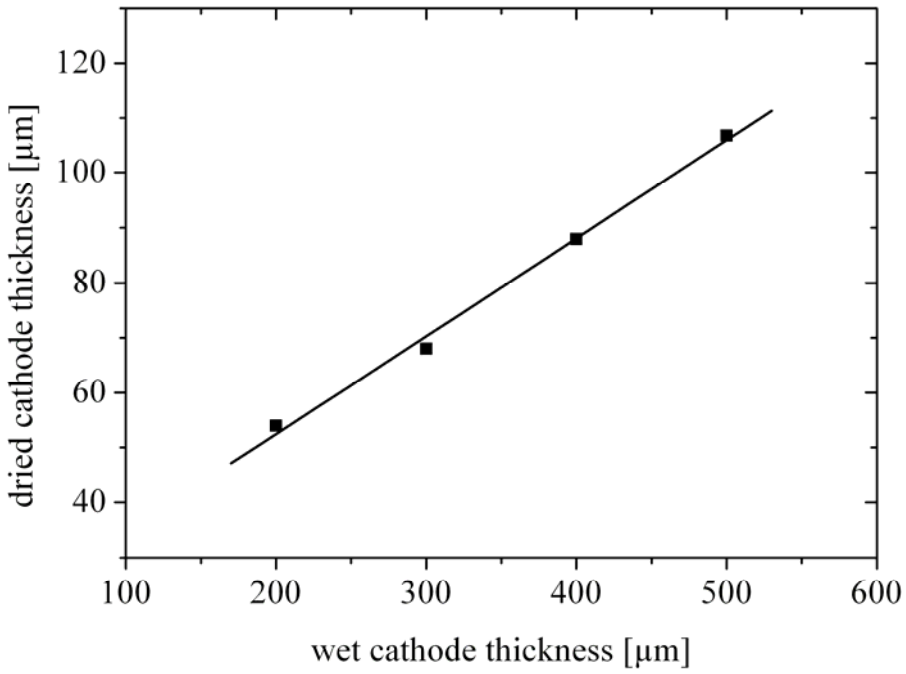

Figure S8. Linear dependence of the cathode thickness in the wet vs. the dried state (doctor blading).