Supporting Information

Para-Nitroaniline-Functionalized Organic-Inorganic Hybrid Materials

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Calculation of molar extinction coeffient

$$\varepsilon = \frac{E}{c \cdot d} = \frac{E \cdot V \cdot M}{m \cdot d} \; ; \left[\frac{L}{mol \cdot cm}\right] \qquad \text{(S1)}$$

E – extinction;

c – molar concentration [L·mol^{-1}]

V – volume of solution used to dissolve the xerogel [L];

m – mass of the dissolved xerogel [g];

d – optical path length [cm];

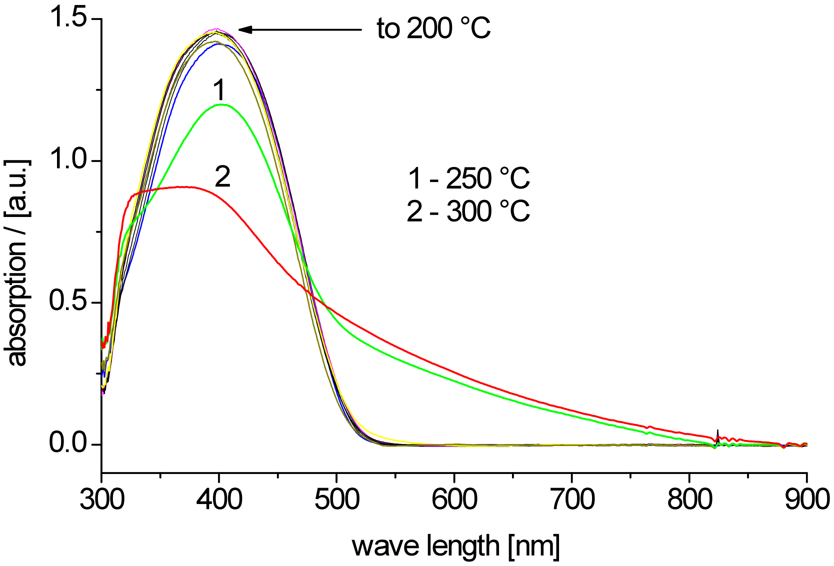
M – molecular weight [g·mol^{-1}])

Thermal stability of xerogels

Table S1: Results of the thermogravimetric analysis (TGA) of various xerogels. Measurements were performed in dry He atmosphere.

sample	heating rate	weight loss 30–200 °C	weight loss 200–500 °C	weight loss to 500 °C / (800 °C)
B1	40 K min^{-1}	3.5 %	10.5 %	14.0 %
	40 K min^{-1}	3.8 %	10.5 %	14.3 % / (20.1 %)
B4	40 K min^{-1}	4.0 %	10.8 %	14.8 %
B10	40 K min^{-1}	4.4 %	10.4 %	14.8 %
	10 K min^{-1}	3.9 %	10.1 %	14.0 %
B12	40 K min^{-1}	2.8 %	10.2 %	13.0 %

Figure S1: UV/Vis absorption spectra of *p*-nitroaniline functionalized xerogels heat treated for five hours at temperatures of up to 300 °C. Measurements were performed in reflectance technique.



Influence of pH value on optical properties of the chromophoric system

Figure S2: Shift in UV/Vis absorption wavelength of the chromophoric system of p-nitroaniline xerogels with changes in pH. Xerogels were dissolved completely using 1M NaOH and titration was performed using hydrochloric acid.

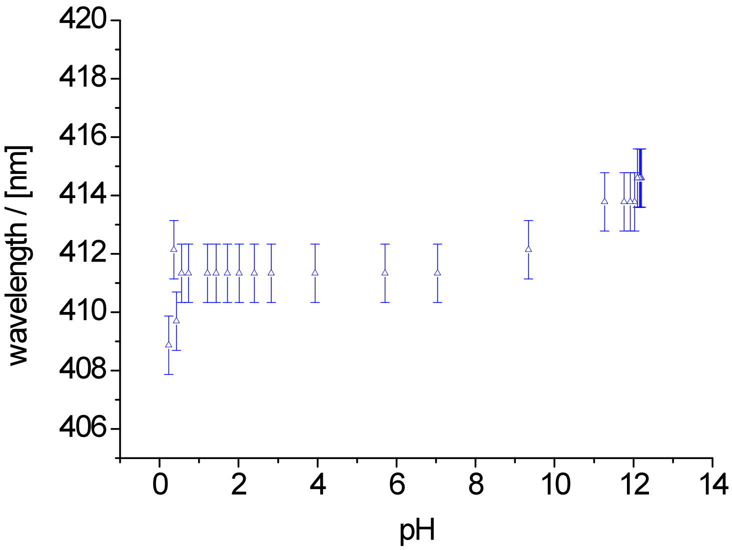


Figure S3: Representative ^{13}C-$\{^{1}$H$\}$-CP-MAS NMR spectrum of *p*-nitroaniline functionalized xerogels based on the diaminofunctionalized trialkoxysilane DAS and TEOS (molar ratio of 1:10). The chemical structures of the mono- and disubstituted (left side) products as well as their assignment to the observed signals are shown. Signals 5 and 10 (60 ppm and 19 ppm) originate from non-hydrolyzed ethoxy groups of TEOS, signal 8 (30 ppm) from adsorbed acetone. The magic angle spinning (MAS) frequency was set to 12.5 kHz.

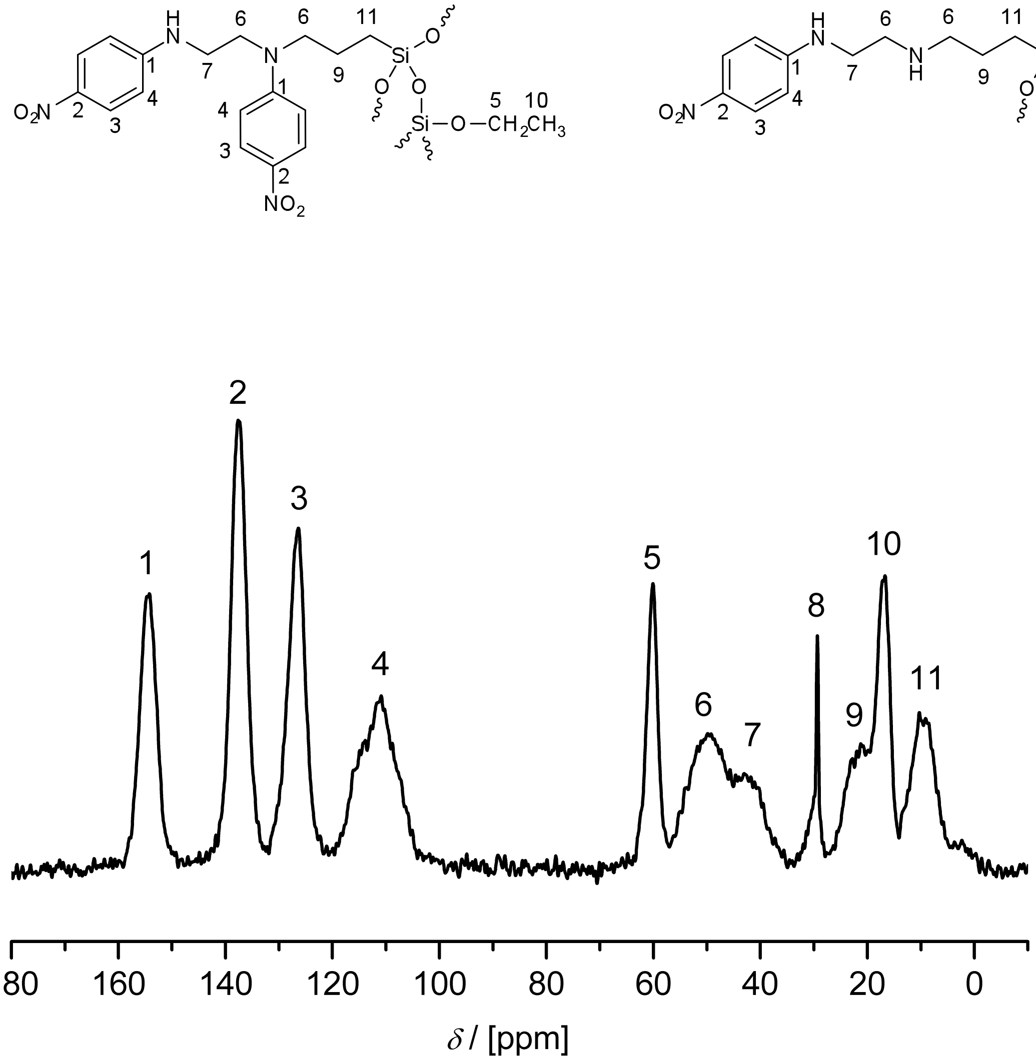


Figure S4: Representative ^{13}C-$\{^1H\}$-CP-MAS-NMR spectrum of *p*-nitroaniline functionalized xerogels based on the triaminofunctionalized trialkoxysilane TAS and TEOS (molar ratio of 1:10), and molecular structure of the most likely di-substituted product. Mono-, di-, or trisubstituted products cannot be distinguished in the spectrum. Signal 7 (30 ppm) originates from adsorbed acetone. The MAS frequency was set to 12.5 kHz. The structure of the disubstituted product is shown.