SUPPLEMENTARY INFORMATION

Tunable functional coverage of biocompatible magnesium silicate nanotubes by microwave-assisted silanization

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Calibration of the ninhydrin optical response

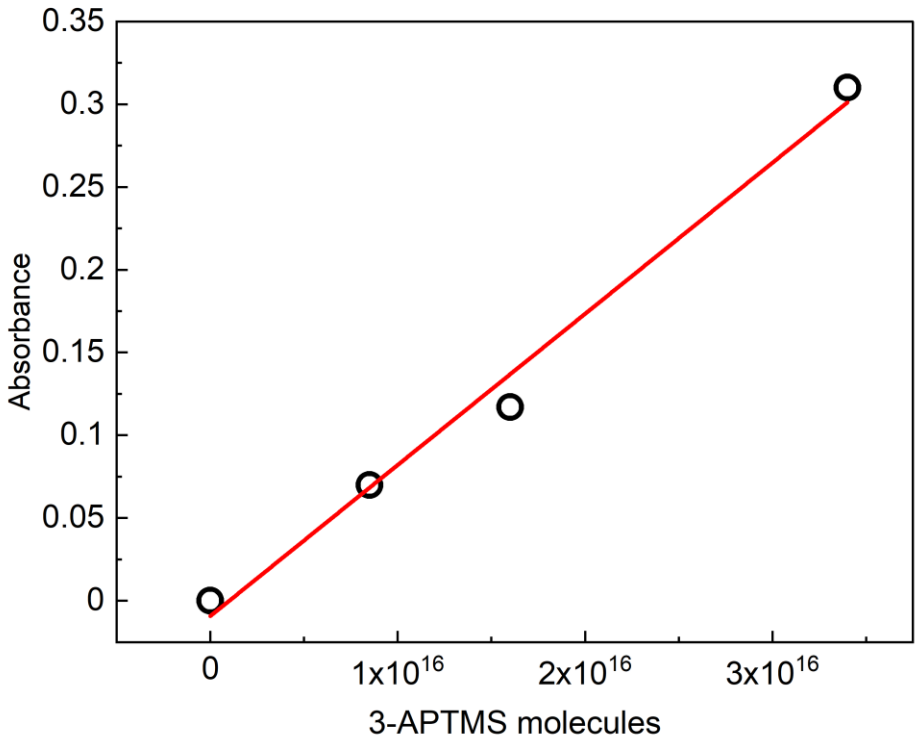

Figure S1 3-APTMS calibration curve performed by measuring the absorbance at $\lambda = 588$ nm of increasing numbers of 3-APTMS molecules. The molar extinction coefficient is calculated as the slope of the straight line $\varepsilon = (y_2 - y_1)/(x_2 - x_1)$ where y are the absorbance values and x are the number of 3-APTMS. $\varepsilon = 9.12\times10^{-18}$ (cm×M)$^{-1}$.

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TEM images of isolated NTs

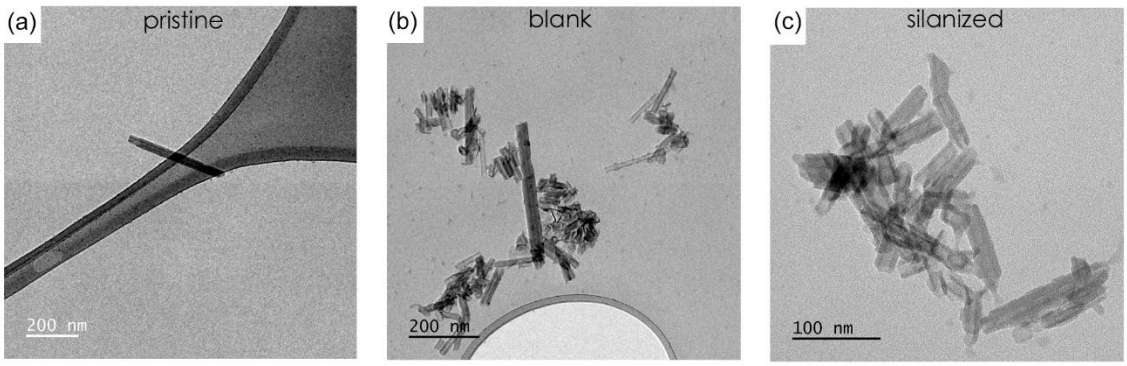

Figure S2 Bright-filed TEM images of as synthesized NTs (a) and after MW-assisted treatment with (c) and without (b) 3-APTMS silanizing agent, deposited from isopropanol on lacey C-coated Cu-grids.

TGA characterization

To estimate the amount of hydroxyl groups on the surface of bare NTs, thermogravimetric analysis (TGA) was employed. The weight loss observed in the temperature range of 150–1000 °C ($\Delta W_{150\text{-}1000°C}$, Fig. S3 and S4) was attributed to the desorption of water resulting from the recombination of two surface –OH groups. The following equation was used for this estimation:

$$\Delta w_{150\text{-}1000°C} = \frac{1}{2}\, n_{OH}\, MW_{H_2O} \tag{S1}$$

where n_{OH} are the moles of surface hydroxyl groups and MW_{H_2O} is the molecular weight of water. The amount of OH groups available onto bare NTs can be calculated:

$$w\%_{OH} = \frac{n_{OH}\, MW_{OH}}{w_{NTs(150°C)}} 100 = \frac{2\Delta w_{150\text{-}1000°C}\, MW_{OH}}{MW_{H_2O}\, w_{NTs(150°C)}} 100 \tag{S2}$$

Where MW_{OH} is the molecular weight of OH groups and $w_{NTs(150°C)}$ is the weight of the sample after drying at 150 °C, necessary to remove the physisorbed species as solvent molecules.

The increased weight loss observed in the functionalized NTs sample within the temperature range of 150–1000 °C is attributed to several processes:

(i) the combustion of the $-CH_2CH_2CH_2NH_2$ functional group derived from 3-APTMS, which is covalently anchored to the NTs surface;

(ii) water desorption resulting from the recombination of surface –OH groups, assuming that each 3-APTMS molecule is bound to the surface via two hydroxyl groups;

(iii) desorption of water originating from –OH groups formed by the hydrolysis of the third ethoxy group of 3-APTMS, which does not participate in bonding with the NTs surface.

The following equation was used to determine the degree of functionalization:

$$\Delta W_{150\text{-}1000°C} = n_F \cdot MW_F + \frac{1}{2} \cdot \left(n_{OH} \cdot w_{NTs(1000°C)} - 2n_F\right) \cdot MW_{H_2O} + \frac{1}{2} \cdot \left(n_{OH\text{-}APTMS} \cdot MW_{H_2O}\right) \tag{S3}$$

where n_F represents the number of moles of 3-APTMS grafted onto the NTs surface, MW_F (58.0 g mol^{-1}) is the molecular weight of the $-CH_2CH_2CH_2NH_2$ group derived from 3-APTMS and anchored to the NTs, n_{OH} is the total number of hydroxyl groups per gram of NTs, previously determined by TGA (Eq. S1) and equal to 18 mmol g^{-1}. $w_{NTs(1000°C)}$ is the weight of the sample at 1000 °C. $n_{OH\text{-}APTMS}$ denotes the number of moles of hydroxyl groups bonded to 3-APTMS (equal to n_F under the assumption that each 3-APTMS molecule is attached via a bi-dentate bond). The factor ½ accounts for the condensation reaction, in which two hydroxyl groups combine to release one molecule of water. This same equation, with minor modifications, has also been applied to calculate n_F in cases where 3-APTMS forms either mono- or tri-dentate bonds.

From Eq. S3, n_F is than used to calculate the amount of 3-APTMS grafted onto NTs ($w\%_{APTMS}$, Fig. S4) and the number of 3-APTMS molecules anchored per squared nanometres of surface of NTs (σ, Fig. S5):

$$w\%_{APTMS} = \frac{n_F \cdot MW_F}{w_{NTs(1000°C)}} 100 \tag{S4}$$

$$\sigma\ [\text{number molecules/nm}^2] = \frac{n_F\ [\text{mol}] \cdot N_A\ [\text{number/mol}]}{w_{NTs(1000°C)}[\text{g}] \cdot SSA\ [\text{m}^2/\text{g}] \cdot 10^{18}[\text{nm}^2/\text{m}^2]} \quad \text{(S5)}$$

where N_A the Avogadro number, SSA the specific surface area of NTs ($SSA = 147 \pm 3\ m^2\ g^{-1}$, see BET isotherm in Figure 4d).

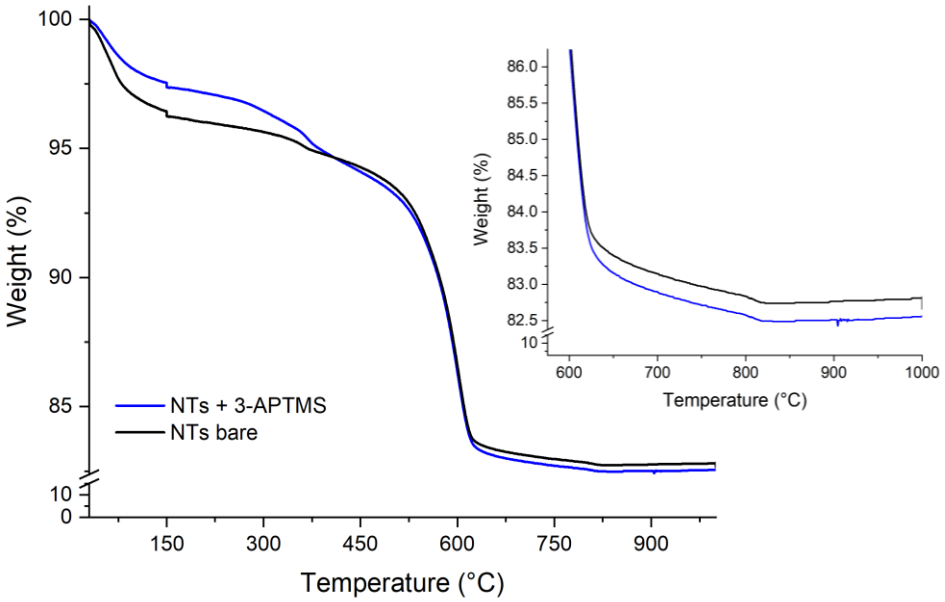

Figure S3 Weight loss as a function of temperature in bare NTs (black curve) and functionalized NTs. The inset shows an enlarged view within the temperature range 600–1000 °C.

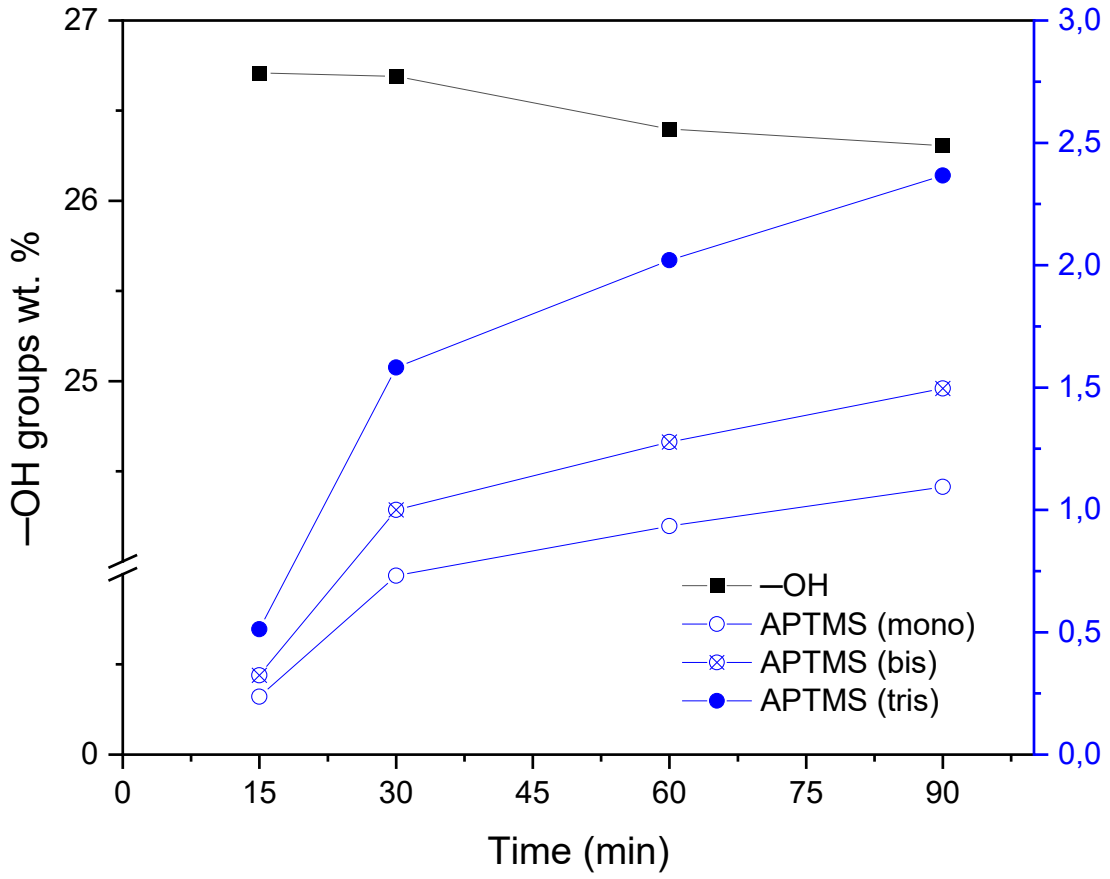

Figure S4 Weight fraction of -OH groups (black symbols) and weight fraction of 3-APTMS (blue symbols) as a function of treatment time calculated from the TGA results obtained from NT samples corresponding to the same series reported in Fig. 9.

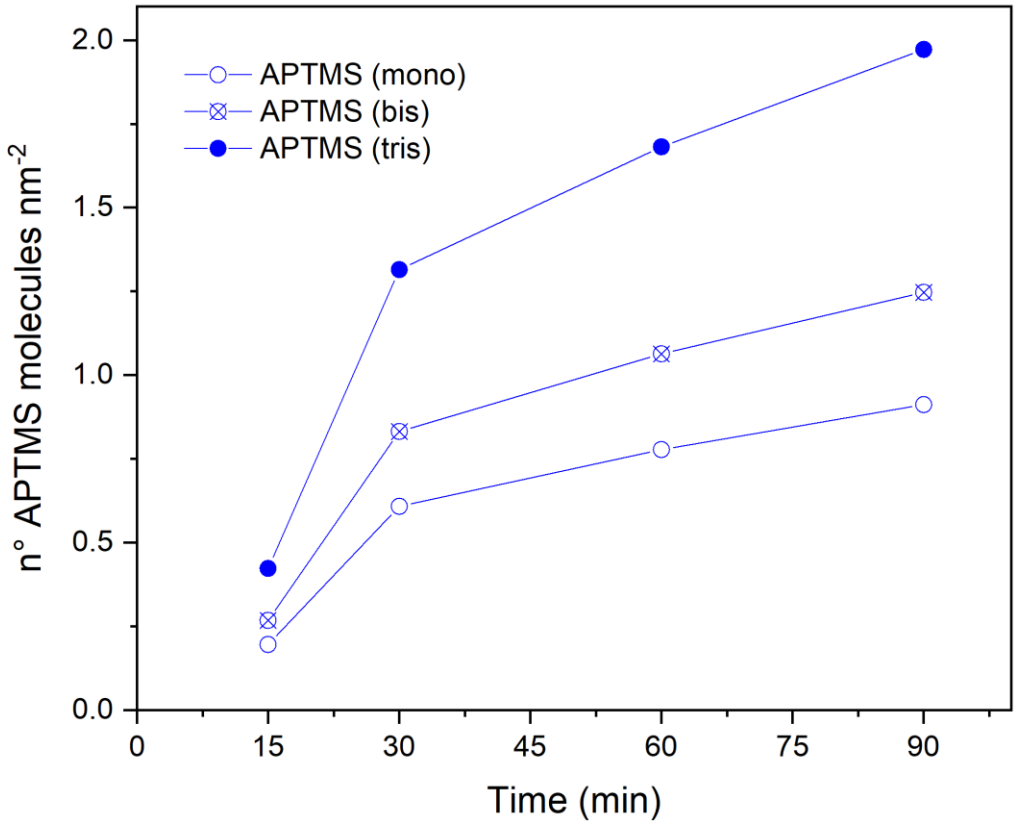

Figure S5 Number of bonded silane molecules per square nm as deduced from the TGA of NT samples corresponding to the same series reported in Fig. 9 and assuming mono-, bi, and tri-dentate bonding.