Supplementary Information (SI) for Nanoscale.
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Supporting Information for:

Room Temperature Sonochemically-Initiated Dehydrogenative Coupling of Silanes on Silicon Nanoparticle Surfaces

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Surface Coverage

Thermal Gravimetric Analysis (TGA) was used to characterize the degree of functionalization of the Si NPs described. The output of this analysis technique is a percentage of the total mass loss over a temperature range, which is independent of particle size, surface characteristics, or ligand used. To properly compare the extent of functionalization between different nanoparticle sizes, this mass loss must be converted to surface coverage, which was done with the following procedure:

1. The amount of Si atoms present were calculated, expressed in the number of Si atoms present per nm, utilizing the density and atomic mass of Si, as well as Avogadro's number
2. Assuming a 'surface radius' that is one Si atom thick, the number of atoms that are on the surface of the particle were calculated, and assuming the surface Si atoms average out to being SiH_2, the number of available surface sites to react with are twice the number of surface atoms.
3. Based on the ligand used (e.g. dodecene), the molecules that were lost in the course of TGA were calculated using the mass loss and the molar mass of the ligand
4. The theoretical number of silicon particles that would be present in the analyzed sample can be determined from the Si/nm^3 from (1), with an additional option for tuning the accuracy of the calculation – the surface of the SI NPs are likely to be somewhat oxidized, and thus not all SiH_x, so some amount of SiO_2 can be accounted for by using a corrected molar mass term via a weighted average calculation.
5. The surface coverage can then be calculated from the molecules of ligand lost per Si NP (step 3 / step 4), and the number of reactive sites (step 2).

$$\frac{\#\ Si\ Atoms}{nm^3} = \frac{Density\left(\frac{g}{nm^3}\right)}{Molar\ Mass\left(\frac{g}{mol}\right)} * N_A\left(\frac{atoms}{mol}\right) \quad (1)$$

$$\# \, Surface \; Reactive \; Sites = \frac{4}{3}\pi\left(r^3 - \left(r - r_{Si)}\right)^3\right) * \frac{\# \, Si \; Atoms}{nm^3} * 2 \tag{2}$$

$$Molecules \; of \; Ligand \; Lost = \frac{Mass \; Loss \; (g)}{Molar \; Mass \left(\frac{g}{mol}\right)} * N_A \tag{3}$$

$$Theoretical \; Particle \; Count = \frac{\frac{\# \, Si \; Atoms}{nm^3}}{N_A} * V_{Particle} * Molar \; Mass_{corr.} \tag{4}$$

$$\% \; Surface \; Coverage = \frac{\frac{Molecules \; of \; Ligand \; Lost}{Theoretical \; Particle \; Count}}{\# \, Surface \; Reactive \; Sites} \tag{5}$$

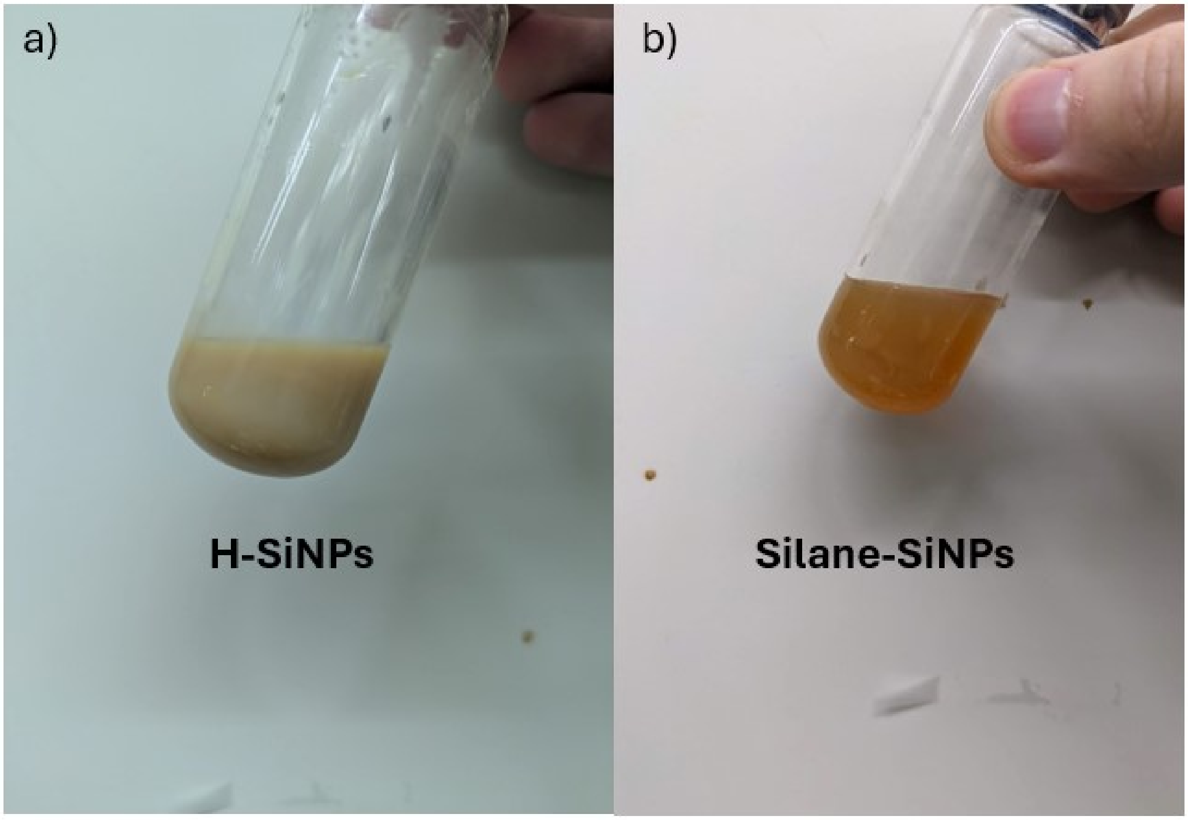

Figure S1: a) Opaque hydrogen-terminated SiNPs (6 nm) compared to b) semi-transparent silane-SiNPs (6 nm)

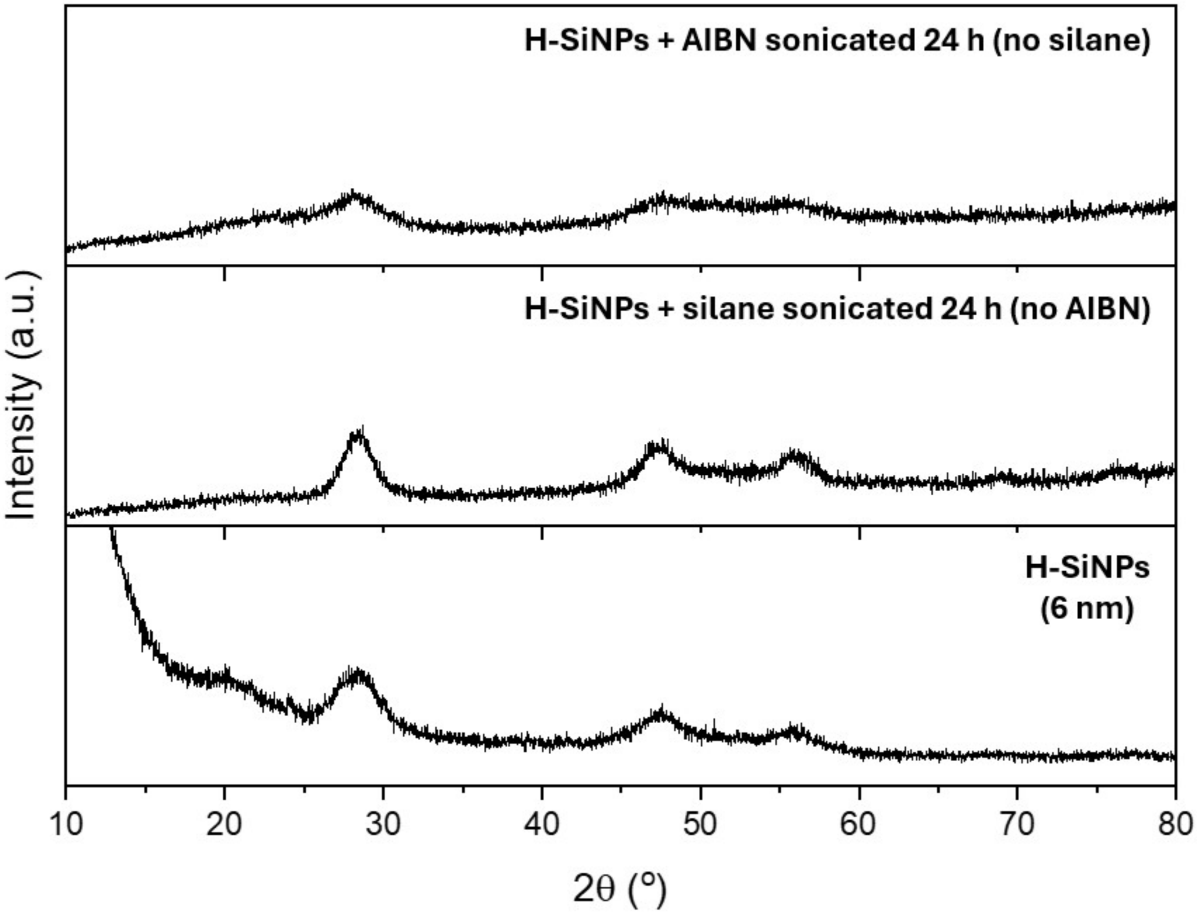

Figure S2: XRD spectra of control reactions – H-SiNPs and the products of their sonication with radical initiator or silane in isolation.

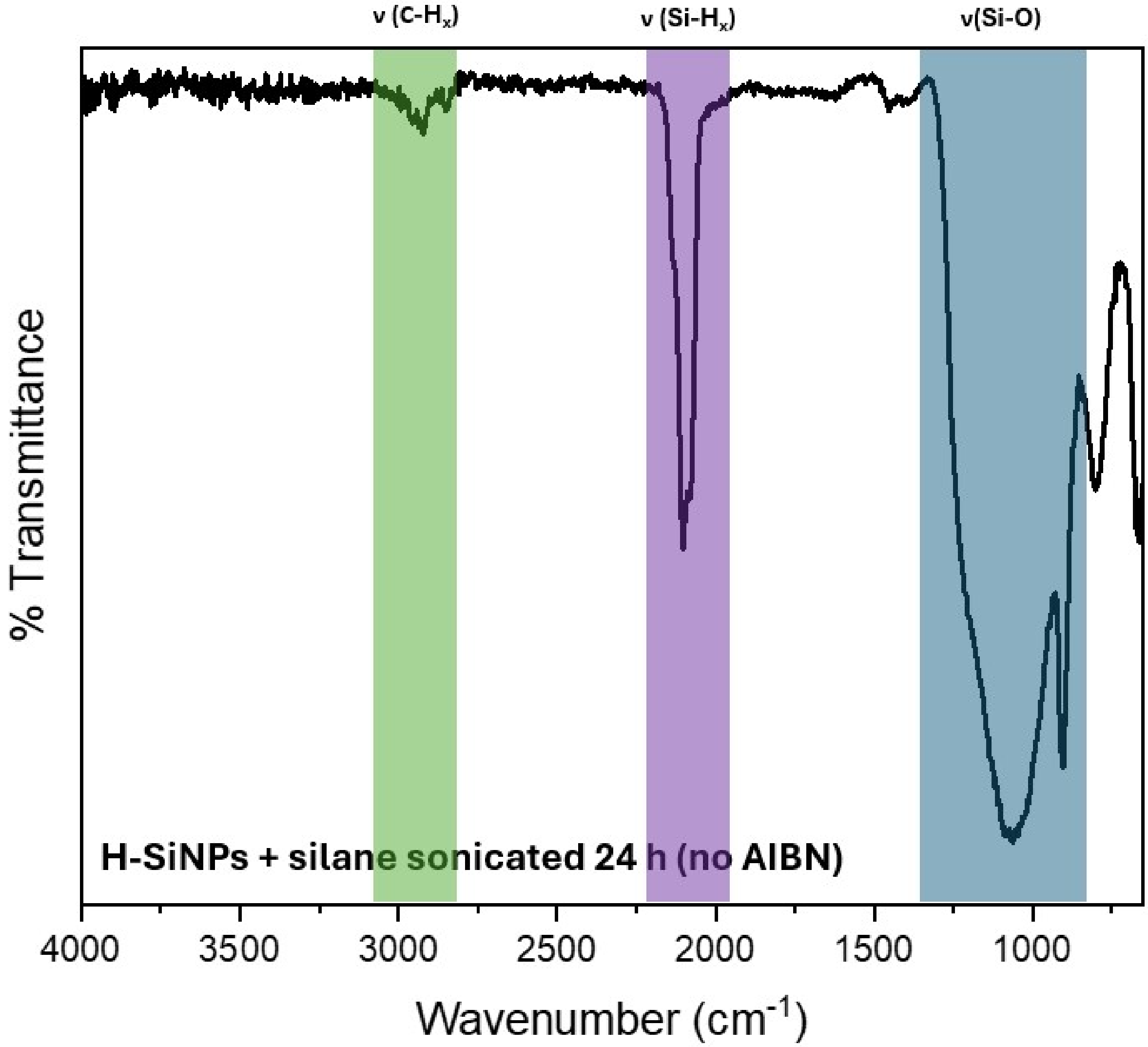

Figure S3: FT-IR spectrum of 6 nm H-SINPs reacted with dodecylsilane in the absence of radical initiator

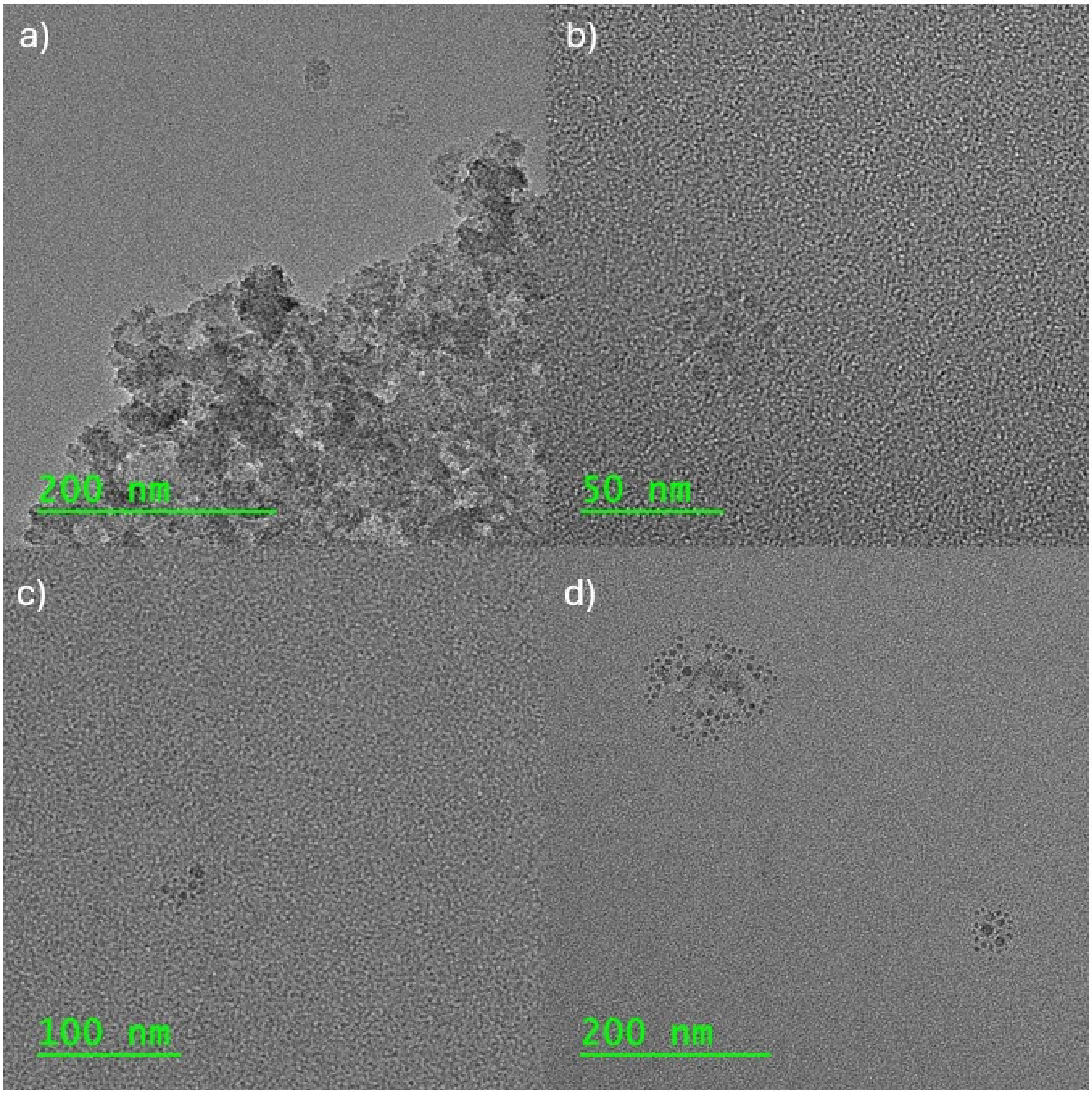

Figure S4: Bright-Field TEM images of 6 nm SiNPs functionalized with a) dodecylsilane, b) and d) trioctylsilane, and c) diisopropylsilane.

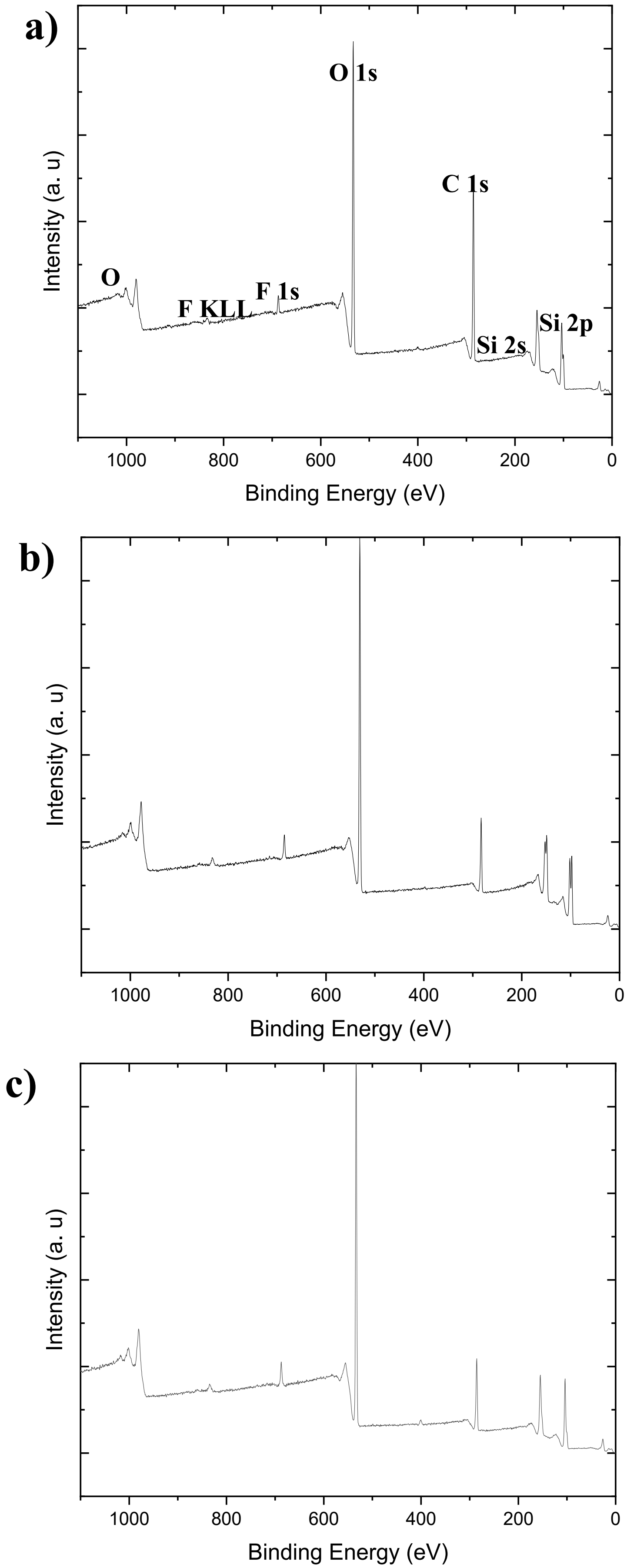

Figure S5: Survey XP spectra of a) dodecylsilane-, b) diisopropylsilane-, and c) trioctylsilane- SiNPs

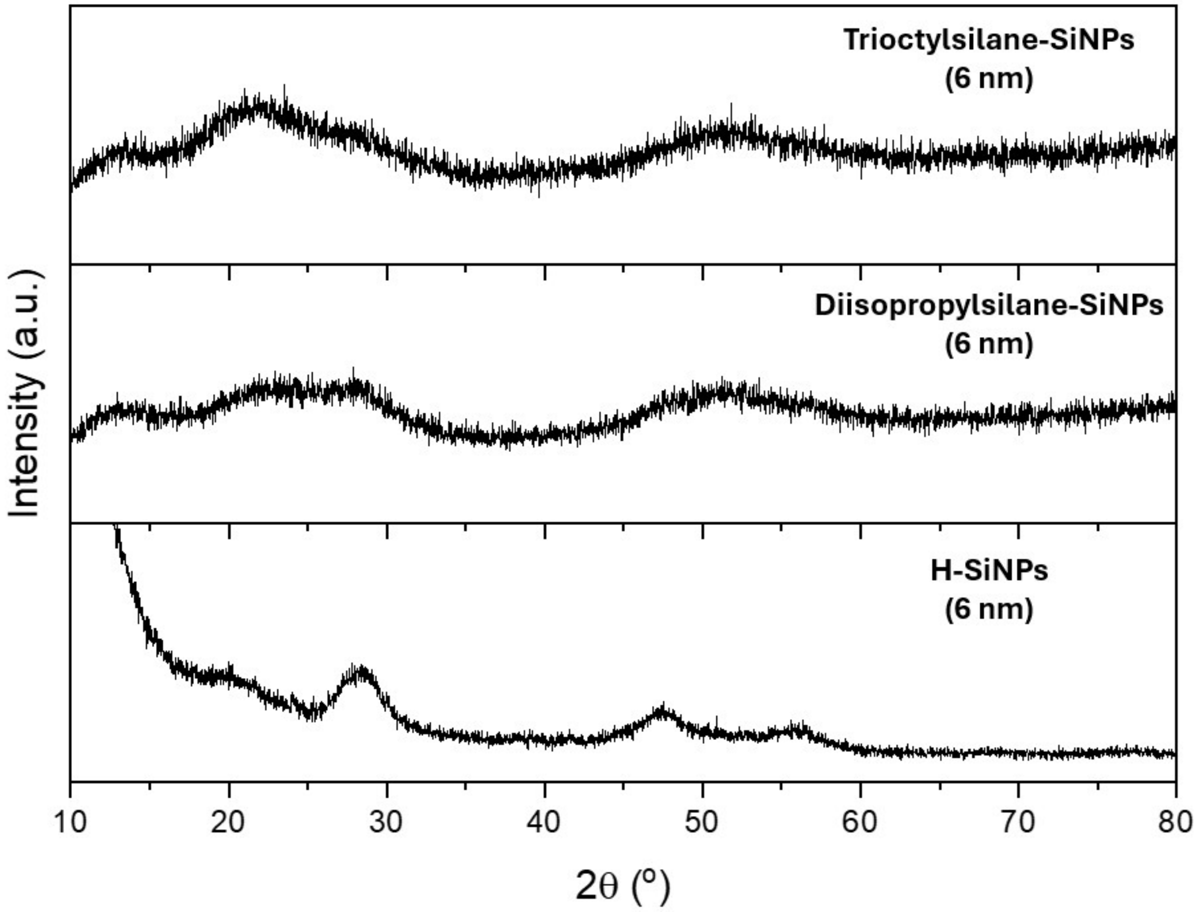

Figure S6: XRD patterns of diisopropyl- and trioctyl-SiNPs functionalized via radically-induced sonochemical dehydrocoupling.

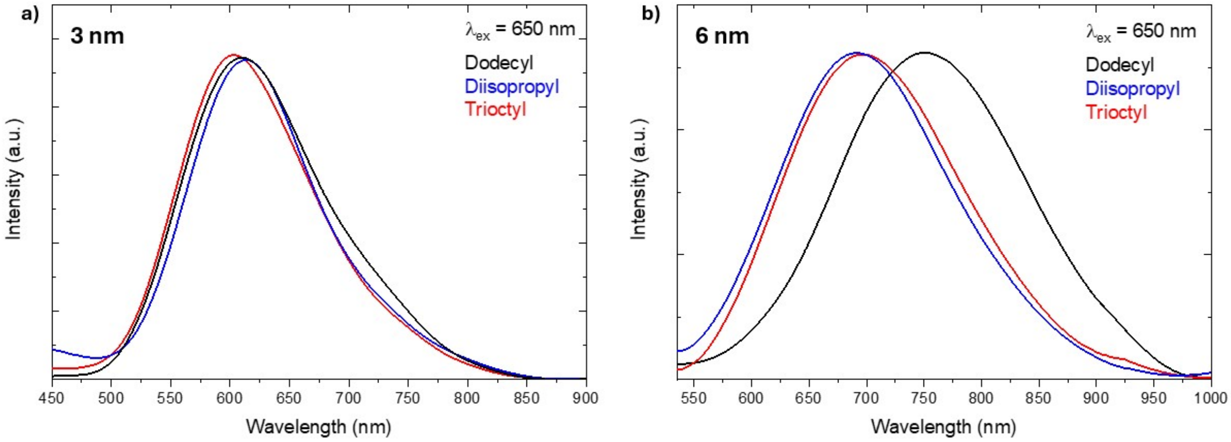

Figure S7: Normalized photoluminescence spectra of a) 3 and b) 6 nm silane-SiNPs sonicated for 24 h with AIBN.

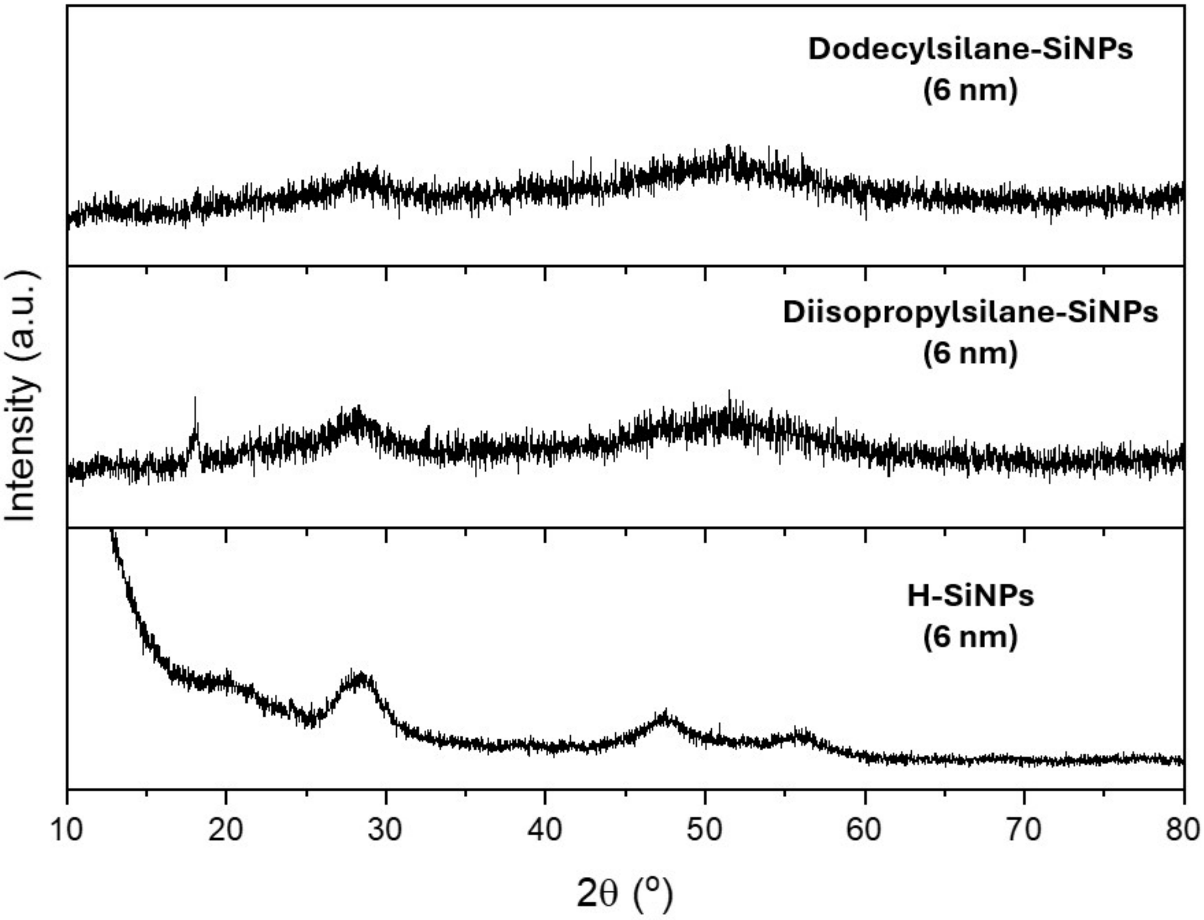

Figure S8: XRD patterns of 6 nm silane-SiNPs functionalized via thermal (80 °C) dehydrocoupling for 24 h.

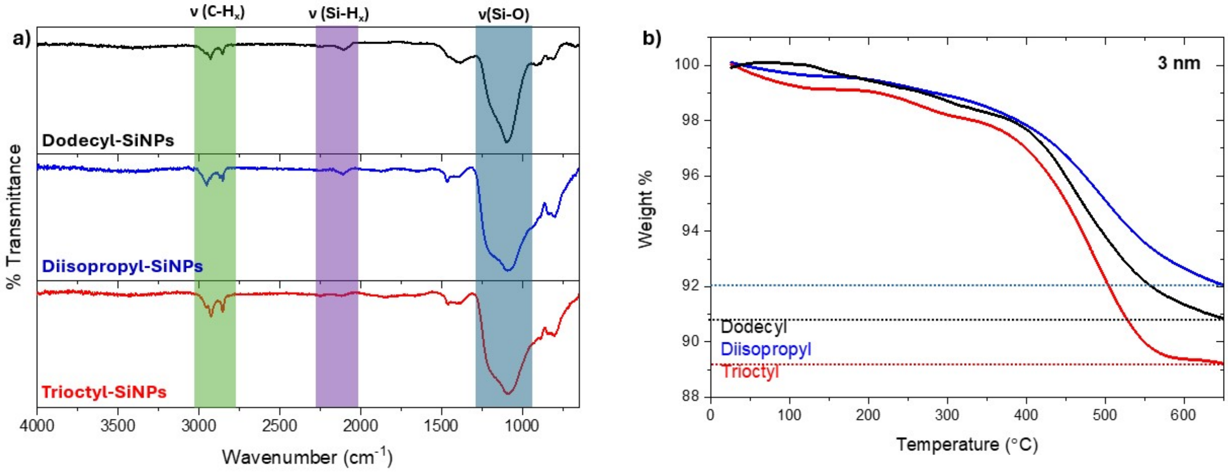

Figure S9: a) FT-IR and b) TGA of 3 nm silane-SiNPs functionalized via sonochemical dehydrocoupling for 24 h in the presence of AIBN.

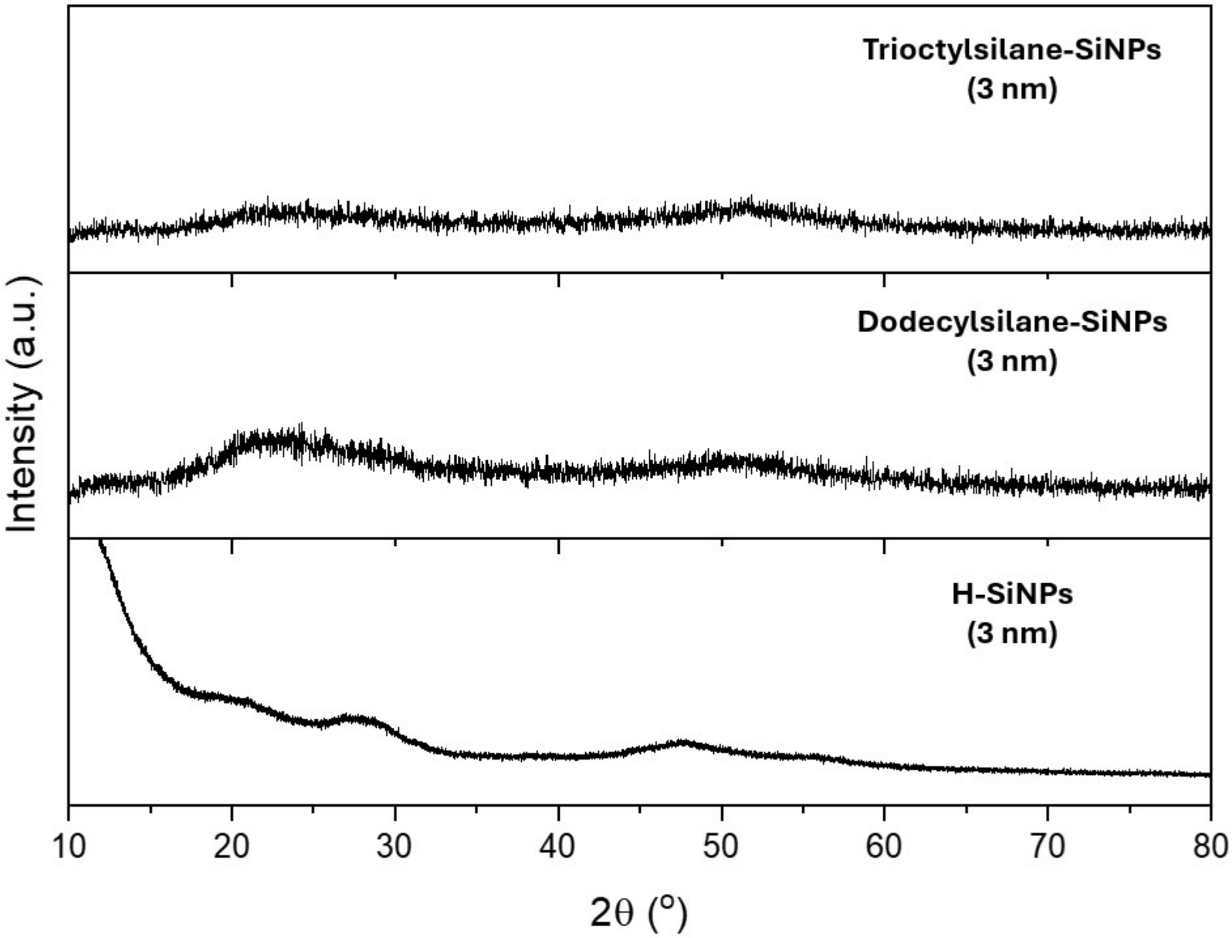

Figure S10: XRD patterns of 3 nm silane-SiNPs functionalized via sonochemical dehydrocoupling for 24 h in the presence of AIBN.

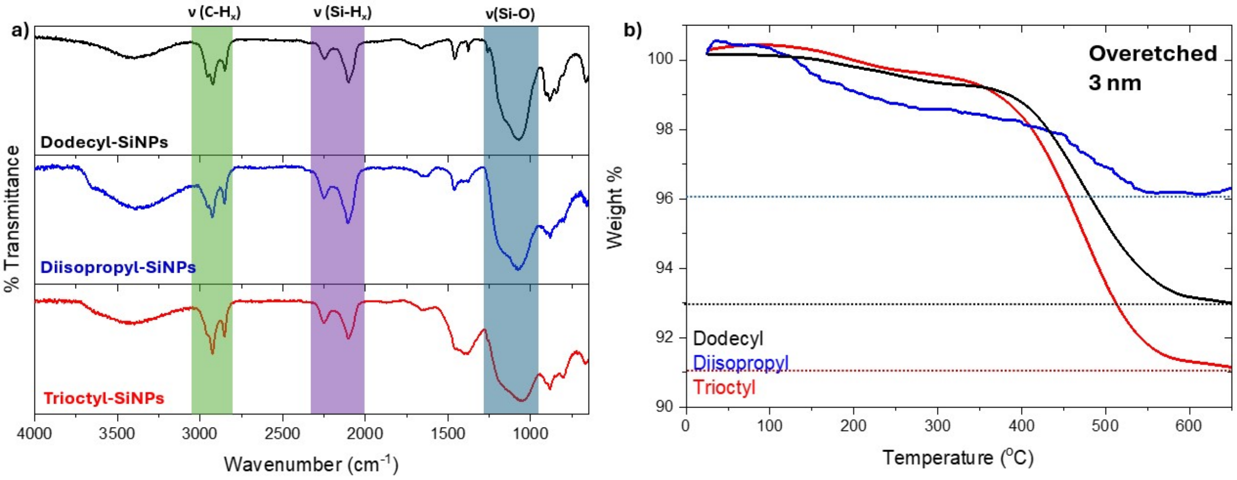

Figure S11: a) FT-IR and b) TGA of overetched 3 nm silane-SiNPs functionalized via sonochemical dehydrocoupling for 24 h in the presence of AIBN.

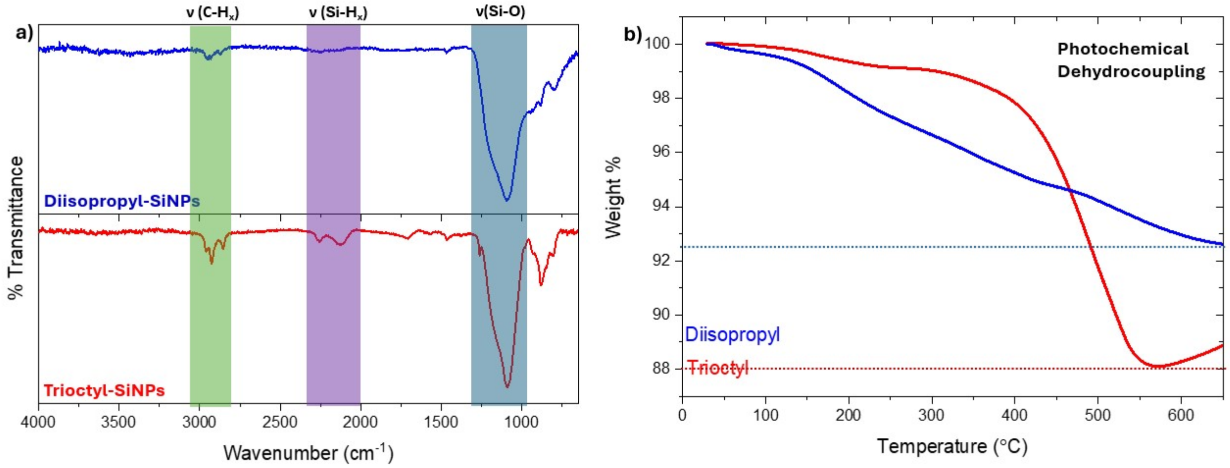

Figure S12: a) FT-IR and b) TGA of 3 nm silane-SiNPs functionalized via photochemical dehydrocoupling (360 nm).