

Supporting information for: Photostability of thermally-hydrosilylated silicon quantum dots

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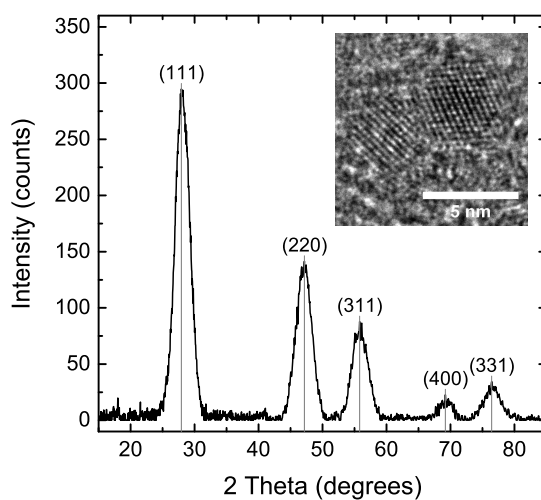


Figure S1: XRD pattern and TEM image (inset) of 4.2 nm SiNCs.

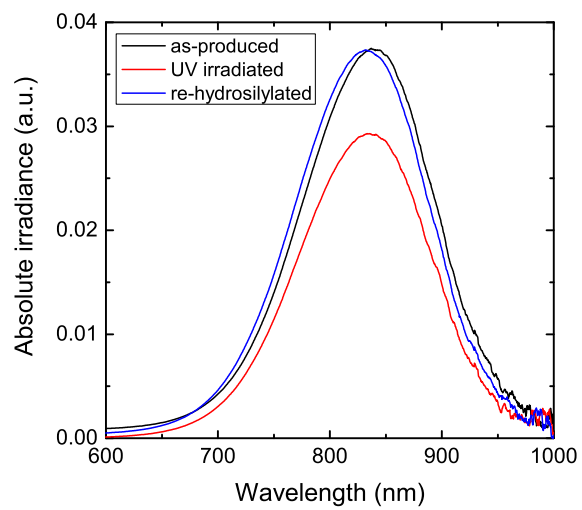


Figure S2: Emission spectra of the as-produced SiNCs (black), UV irradiated SiNCs (red), and re-hydrosilylated SiNCs (blue) normalized to their absorption intensities.

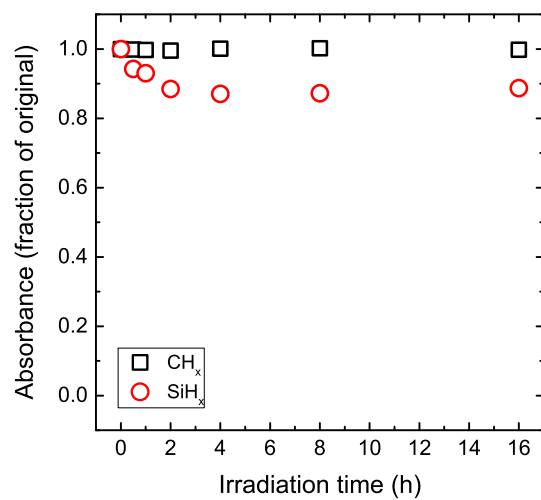


Figure S3: Time evolution of IR absorbance of CH_x and SiH_x groups during photobleaching on the ATR crystal.

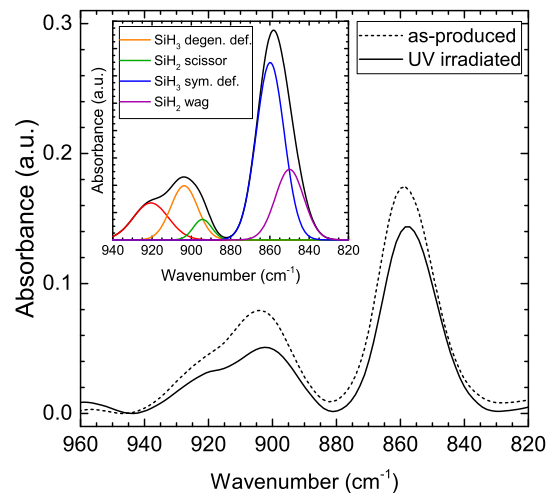


Figure S4: FT-IR spectra of the SiH_x rotational modes of as-produced (dotted black) and UV irradiated (solid black) SiNCs. The inset displays the deconvoluted spectrum, showing SiH₃ degenerate deformation (orange), SiH₂ scissoring (green), SiH₃ symmetrical deformation (blue), and SiH₂ wagging (purple) modes.

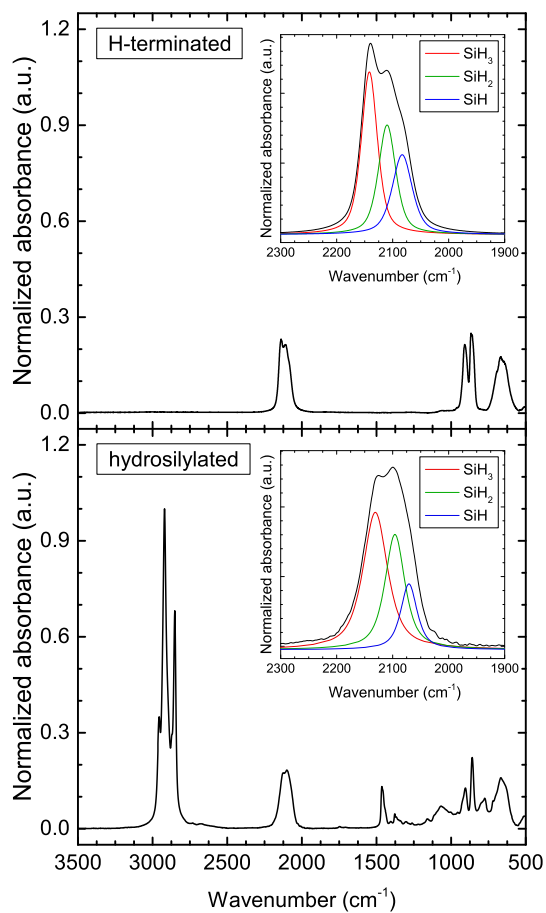


Figure S5: Typical FT-IR spectra of H-terminated SiNCs (top) and thermally-hydrosilylated SiNCs (bottom). Insets show deconvoluted spectra of the silicon hydride stretching modes: SiH₃ (red), SiH₂ (green) and SiH (blue).

Figure S6: Deconvolution of SiH_x stretching modes

Origin (OriginLab, Northampton, MA) was used to deconvolute the SiH, SiH₂, and SiH₃ stretching modes. The three peaks were fitted using the Pseudo-Voigt function with a combination of 60 % Gaussian and 40 % Lorentzian functions.

The peak centers of the SiH, SiH₂, and SiH₃ modes were fixed at 2130 cm⁻¹, 2096 cm⁻¹, and 2070 cm⁻¹, respectively, and the peak widths were allowed to deviate from 30 cm⁻¹ to 50 cm⁻¹. The width of the SiH mode was determined to be 39 cm⁻¹, the width of the SiH₂ mode was 40 cm⁻¹, and the width of the SiH₃ mode was 47 cm⁻¹. The amplitude of the fitted profiles of the SiNCs were determined via the Origin peak fitting tool. The coefficients of determination, R₂, were used to determine quality of fits; all fits possessed R₂ values above 0.99.

To compare the as-produced to the irradiated SiNCs, the CH_x peaks of the two samples were used as references (the organic ligands are stable against UV irradiation as determined from in-situ FT-IR spectroscopy). The peak areas of the SiH_x modes were normalized to the integrated areas of their respective CH_x modes. The absorbance of the SiH, SiH₂, and SiH₃ modes were then normalized to the total SiH_x absorbance of the as-produced SiNCs.