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Supporting Information

Synthesis of Silicon Quantum Dots using Cyclohexasilane (Si_6H_{12})

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HRTEM of sample 2

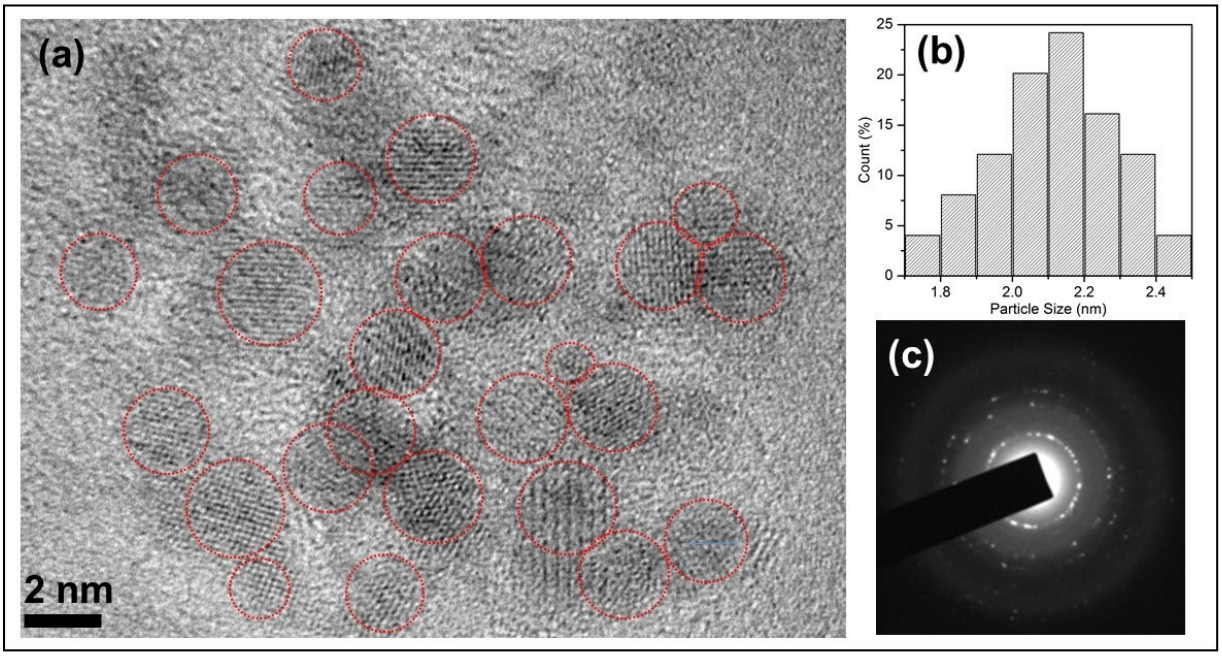

Figure S1. (a) HRTEM images of sample 2 (b) histogram of size distribution of the Si-NCs (sample 2) & (c) Selective area electron diffraction images of 2.

X-ray Photoelectron Spectroscopy

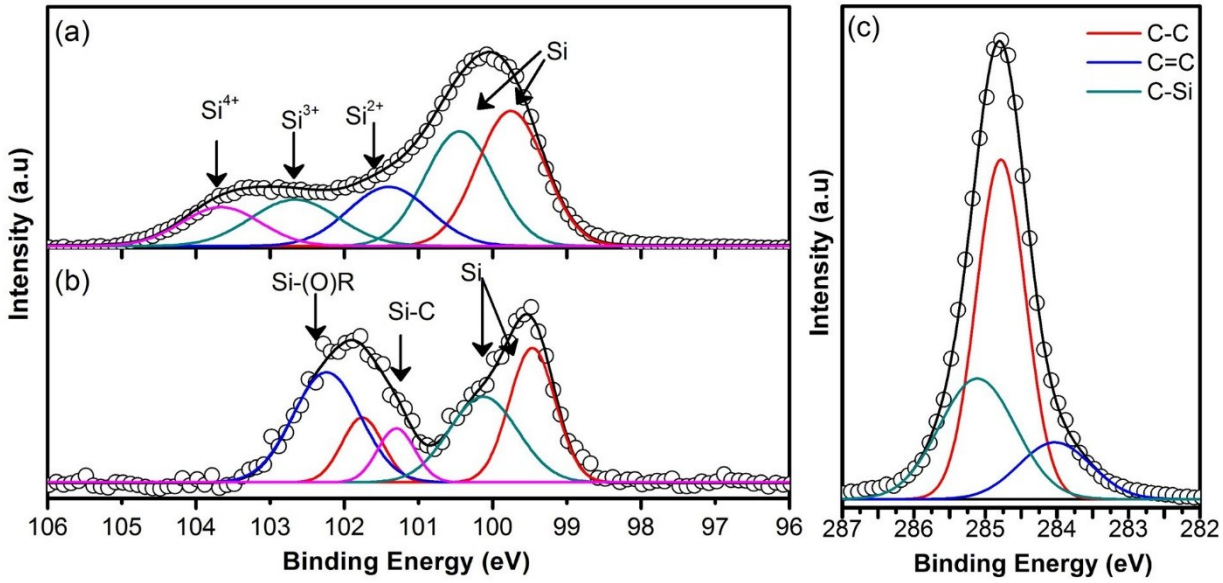

Figure S2. XPS Spectra of sample-1 (a) Si 2p region of as-synthesized sample-1; (b) Si 2p region of hydrosilylated sample-1 and (c) C 1s region of hydrosilylated sample-1. (Dry Si-QDs are smeared on double sided carbon tape, while hydrosilylated Si-QDs (gel) was smeared on gold coated glass substrates).

X-ray photoelectron spectroscopy (XPS) measurements were performed using a Thermo Scientific K-Alpha (Al source) surface analysis tool. Survey and high resolution scans were performed and used to identify the chemical states of the elements. The collected spectra were analyzed (peak fitting) with Avantage Thermo Fisher software. The as-synthesized dry Si-QD powder was applied to sticky carbon tape while the passivated Si-QDs were applied to gold coated glass substrate for XPS analysis. Prior to analysis the analysis chamber was pumped to 10^{-9} mbar and an Ar cluster gun was used to clean the surface contamination.

The Si 2p spectra of as-synthesized and hydrosilylated Si-QDs (sample 1) are shown in Figure S2(a) and S1(b), respectively. The as-synthesized Si-QDs show peaks at 99.6 and 100.5 eV corresponding to Si $2p_{1/2}$ and Si $2p_{3/2}$, respectively, characteristic of elemental Si, along with the other oxidized Si species, Si^{1+} (100.4 eV), Si $^{2+}$ (101.9 eV), Si^{3+} (102.6 eV) and Si^{4+} (103.7 eV).[1, 2]. The presence of elemental Si peaks confirm that the sample is made of Si. The broad oxidized peaks suggest the reaction of hydride terminated Si-QDs with environmental oxygen during the transfer and are not present in the Si-QDs intrinsically. Elemental Si peaks akin to as-synthesized samples were noticed for hydrosilylated Si-NCs (Figure S2(b)), along with peaks corresponding to Si-C (101.3 eV) and Si-R/Si(O)R (101.8 & 102.3 eV)[3], with no significant contributions arising from oxidized Si species. The C 1s spectra of hydrosilylated Si-QDs presented in Figure S2(c) depicts the presence of C=C (284.5 eV), C-C (285.1 eV) and C-Si (283.9 eV), respectively[4], with no oxide related peaks, in agreement with Si 2p elemental spectra. This result is in accordance with the FTIR observations and confirms that hydride terminated Si-QDs are passivated with alkyl groups via hydrosilylation.

References

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